

chain nodes :

25 26 27 28 29 30 31 32 36 37 39 40 41 42 43 44 45 46
 47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
 91 92 93 94 95 96

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
 21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69

chain bonds :

2-28 3-95 9-93 10-27 13-37 14-25 20-36 21-26 29-30 31-32
 39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
 47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-96 92-94
 93-94 95-96

ring bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11
 11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19
 18-20 19-22 20-21 21-22 22-24 57-58 57-62 58-59 59-60 60-61
 61-62 64-65 64-69 65-66 66-67 67-68 68-69

exact/norm bonds :

7-8 8-11 12-16 13-37 15-16 20-36 39-40 40-41 41-73 42-43
 43-44 43-74 45-46 45-49 47-48 47-50 47-76 49-75 51-52 51-77
 53-78 54-79 55-81 91-96 92-94

exact bonds :

2-28 3-95 9-93 10-27 14-25 21-26 29-30 31-32 56-57 93-94
 95-96

normalized bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
 12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
 22-24 57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
 66-67

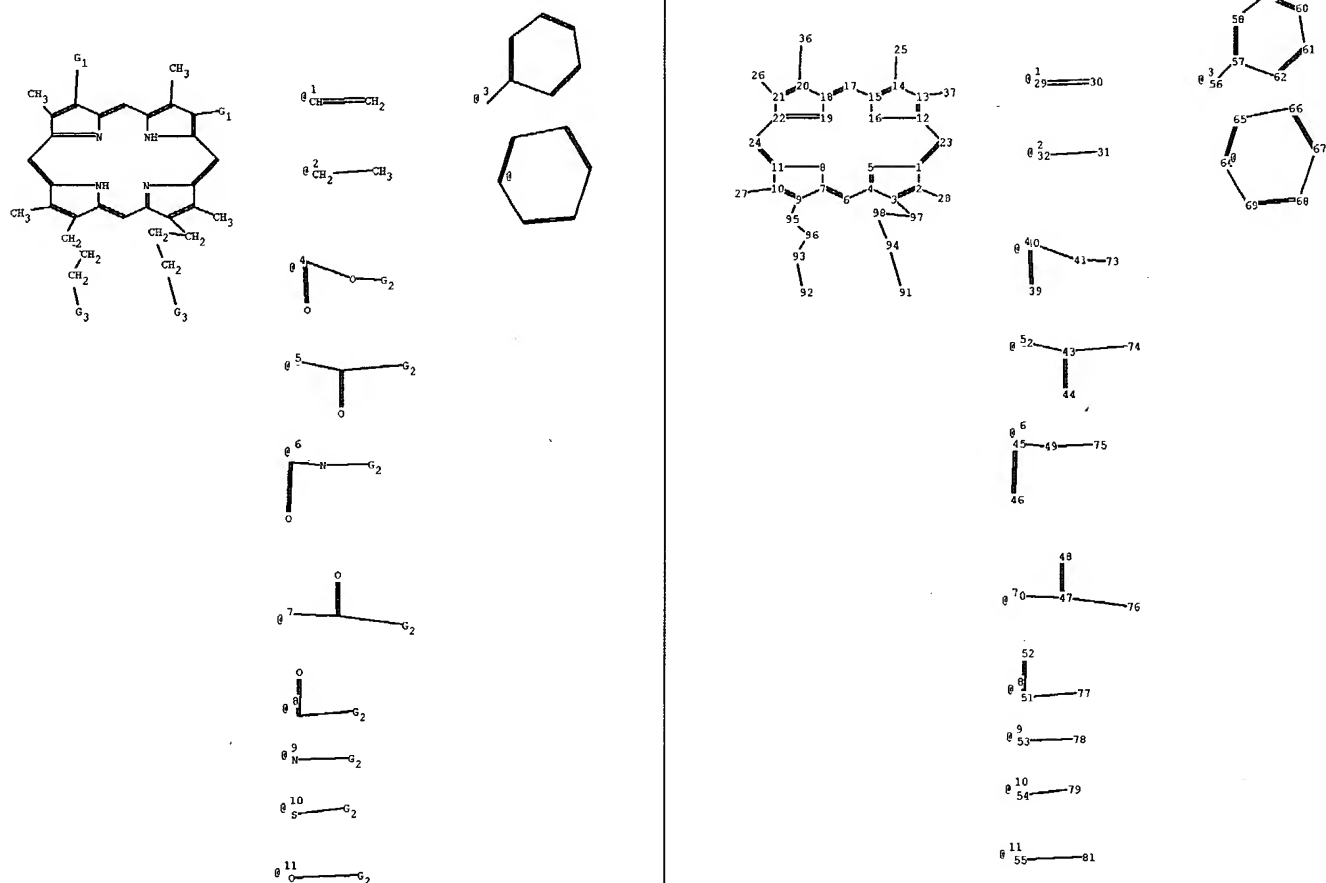
G1: [*1], [*2]

G2: H, CH₃, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*2], [*3]

G3: [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11]

Match level :

1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom
10:Atom	11:Atom	12:Atom	13:Atom	14:Atom	15:Atom	16:Atom	17:Atom	
18:Atom	19:Atom	20:Atom	21:Atom	22:Atom	23:Atom	24:Atom	25:Atom	
26:Atom	27:Atom	28:Atom	29:Atom	30:Atom	31:Atom	32:Atom	36:Atom	
37:Atom	39:CLASS	40:CLASS	41:Atom	42:Atom	43:Atom	44:Atom		
45:CLASS	46:CLASS	47:CLASS	48:CLASS	49:CLASS	50:CLASS	51:CLASS		
52:CLASS	53:CLASS	54:CLASS	55:CLASS	56:CLASS	57:Atom	58:Atom		
59:Atom	60:Atom	61:Atom	62:Atom	64:Atom	65:Atom	66:Atom	67:Atom	
68:Atom	69:Atom	73:CLASS	74:CLASS	75:CLASS	76:CLASS	77:CLASS		
78:CLASS	79:CLASS	81:CLASS	91:CLASS	92:CLASS	93:CLASS	94:CLASS		
95:CLASS	96:CLASS							



chain nodes :

25 26 27 28 29 30 31 32 36 37 39 40 41 42 43 44 45 46
 47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
 91 92 93 94 95 96 97 98

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
 21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69

chain bonds :

2-28 3-97 9-95 10-27 13-37 14-25 20-36 21-26 29-30 31-32
 39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
 47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-94 92-93
 93-96 94-98 95-96 97-98

ring bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11
 11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19
 18-20 19-22 20-21 21-22 22-24 57-58 57-62 58-59 59-60 60-61
 61-62 64-65 64-69 65-66 66-67 67-68 68-69

exact/norm bonds :

7-8 8-11 12-16 13-37 15-16 20-36 39-40 40-41 41-73 42-43
 43-44 43-74 45-46 45-49 47-48 47-50 47-76 49-75 51-52 51-77
 53-78 54-79 55-81 91-94 92-93

exact bonds :

2-28 3-97 9-95 10-27 14-25 21-26 29-30 31-32 56-57 93-96
 94-98 95-96 97-98

normalized bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
 12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
 22-24 57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
 66-67

G1: [*1], [*2]

G2: H, CH₃, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*2], [*3]

G3: [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11]

Match level :

1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom
10:Atom	11:Atom	12:Atom	13:Atom	14:Atom	15:Atom	16:Atom	17:Atom	
18:Atom	19:Atom	20:Atom	21:Atom	22:Atom	23:Atom	24:Atom	25:Atom	
26:Atom	27:Atom	28:Atom	29:Atom	30:Atom	31:Atom	32:Atom	36:Atom	
37:Atom	39:CLASS	40:CLASS	41:Atom	42:Atom	43:Atom	44:Atom		
45:CLASS	46:CLASS	47:CLASS	48:CLASS	49:CLASS	50:CLASS	51:CLASS		
52:CLASS	53:CLASS	54:CLASS	55:CLASS	56:CLASS	57:Atom	58:Atom		
59:Atom	60:Atom	61:Atom	62:Atom	64:Atom	65:Atom	66:Atom	67:Atom	
68:Atom	69:Atom	73:CLASS	74:CLASS	75:CLASS	76:CLASS	77:CLASS		
78:CLASS	79:CLASS	81:CLASS	91:CLASS	92:CLASS	93:CLASS	94:CLASS		
95:CLASS	96:CLASS	97:CLASS	98:CLASS					

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptaul29pxo

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS	4	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAPLUS
NEWS	5	FEB 05	German (DE) application and patent publication number format changes
NEWS	6	MAR 03	MEDLINE and IMEDLINE reloaded
NEWS	7	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	8	MAR 03	FRANCEPAT now available on STN
NEWS	9	MAR 29	Pharmaceutical Substances (PS) now available on STN
NEWS	10	MAR 29	WPIFV now available on STN
NEWS	11	MAR 29	No connect hour charges in WPIFV until May 1, 2004
NEWS	12	MAR 29	New monthly current-awareness alert (SDI) frequency in RAPRA
NEWS	13	APR 26	PROMT: New display field available
NEWS	14	APR 26	IFIPAT/IFIUDB/IFICDB: New super search and display field available
NEWS	15	APR 26	LITALERT now available on STN
NEWS	16	APR 27	NLDB: New search and display fields available
NEWS	EXPRESS		MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
NEWS	HOURS		STN Operating Hours Plus Help Desk Availability
NEWS	INTER		General Internet Information
NEWS	LOGIN		Welcome Banner and News Items
NEWS	PHONE		Direct Dial and Telecommunication Network Access to STN
NEWS	WWW		CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 14:24:50 ON 03 MAY 2004

=> file req

SINCE	FILE	TOTAL
-------	------	-------

ENTRY SESSION

7.35

7.35

FILE 'REGISTRY' ENTERED AT 14:45:41 ON 03 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

DICTIONARY FILE UPDATES: 30 APR 2004 HIGHEST RN 678535-01-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

Uploading C:\STNEXP4\QUERIES\867a.str

L1 STRUCTURE UPLOADED

$$\Rightarrow d \mid 11$$

L1 HAS NO ANSWERS

L1	STR
----	-----

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

\Rightarrow s 11

SAMPLE SEARCH INITIATED 14:46:23 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 466 TO ITERATE

100.0% PROCESSED 466 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH ** COMPLETE**

```

PROJECTED ITERATIONS:      8025 TO      10615

```

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> search 11

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.

ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full

FULL SEARCH INITIATED 14:46:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 9800 TO ITERATE

100.0% PROCESSED 9800 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.01

L3 13 SEA SSS FUL L1

=>
Uploading C:\STNEXP4\QUERIES\867b.str

L4 STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l4
SAMPLE SEARCH INITIATED 14:47:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 557 TO ITERATE

100.0% PROCESSED 557 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 9725 TO 12555
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> search l4
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 14:47:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 11654 TO ITERATE

100.0% PROCESSED 11654 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 311.68 319.03

FILE 'CAPLUS' ENTERED AT 14:48:01 ON 03 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available

for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 3 May 2004 VOL 140 ISS 19
FILE LAST UPDATED: 2 May 2004 (20040502/ED)

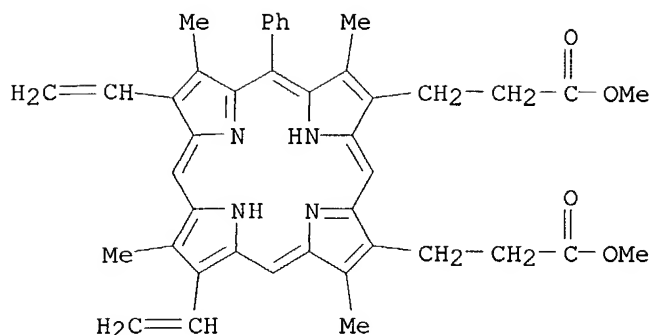
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L7 11 L3

=> d fbib ab hitstr 1-11

L7 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:721210 CAPLUS
DN 134:17340
TI Total synthesis and conformational analysis of monophenyl substituted
protoporphyrins IX
AU Robinsohn, Adriana E.; Maier, Marta S.; Buldain, Graciela Y.
CS Facultad de Farmacia y Bioquímica, Universidad de Buenos Aires, Buenos
Aires, 1113, Argent.
SO Heterocycles (2000), 53(10), 2127-2142
CODEN: HTCYAM; ISSN: 0385-5414
PB Japan Institute of Heterocyclic Chemistry
DT Journal
LA English
OS CASREACT 134:17340
AB The total synthesis of meso-monoaryl protoporphyrins [I; R1 = Ph, R2R3 = H
(II)] and [I; R1R3 = H, R2 = Ph (III)] using a MacDonald type [2+2]
condensation is described. In this method a bisformyl dipyrromethane is
treated with a bis-carboxydipyrromethane. Attempts to obtain the
δ-meso-monoaryl protoporphyrin [I; R1R2 = H, R3 = Ph (IV)] by the
a,c-biladiene method failed as it could not be prepared starting from its
tripyrrene precursor (V). The synthesis of the V is described. Mol.
modeling studies allowed us to find the most favorable conformations for
II and III. In both porphyrins, the exocyclic Ph group adopts a
noncoplanar disposition relative to the plane of the macrocycle. In
porphyrin III the macrocycle is nearly planar while nonplanar saddle
conformation was obtained for porphyrin II.
IT **309757-24-2P**
RL: PNU (Preparation, unclassified); PREP (Preparation)
(attempted preparation of)
RN 309757-24-2 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 8,13-diethenyl-3,7,12,17-
tetramethyl-5-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)



RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1999:367089 CAPLUS

DN 131:110291

TI A convenient synthesis of a Ru(bpy)3-based catenane-type triad and its incorporation into a protein scaffold

AU Hu, Yi-Zhen; Tsukiji, Shinya; Shinkai, Seiji; Hamachi, Itaru

CS Department of Chemistry and Biochemistry, Graduate School of Engineering, Kyushu University, Fukuoka, 812-8581, Japan

SO Chemistry Letters (1999), (6), 517-518

CODEN: CMLTAG; ISSN: 0366-7022

PB Chemical Society of Japan

DT Journal

LA English

AB A catenated heme cofactor consisting of a sensitizer (Ru(bpy)2L (L = I)), a donor (protoheme) II (R = 4'-methyl-2,2'-bipyridin-4-yl) and an acceptor (cyclobis(paraquat-p-phenylene) (III)) was prepared by stepwise coordination, followed by Fe-insertion. Reconstitution of apomyoglobin with this cofactor afforded a protein-based, noncovalently-linked photosynthetic triad.

IT **231302-74-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactant for preparation of iron porphyrinate ruthenium bipyridine bipryidinocrown ether catenated with cyclobisparaquatphenylene for incorporation in protein scaffold)

RN 231302-74-2 CAPLUS

CN Ruthenium(1+), (2,5,8,11,14,27,30,33,36,39-decaoxa-19,22-diazatetracyclo[38.2.2.116,20.121,25]hexatetraconta-16,18,20(46),21,23,25(45),40,42,43-nonaene-κN19,κN22)[8,13-diethenyl-3,7,12,17-tetramethyl-18-[3-[[2-[3-(4'-methyl[2,2'-bipyridin]-4-yl-κN1,κN1')propoxy]ethyl]amino]-3-oxopropyl]-21H,23H-porphine-2-propanoato(1-)](4,4'-dimethyl-2,2'-bipyridine-κN1,κN1')-, (OC-6-43)-, chloride, monohydrochloride, catena compd. with 5,12,19,26-tetraazoniaheptacyclo[24.2.2.22,5.27,10.212,15.216,19.221,24]tetraconta-2,4,7,9,12,14,16,18,21,23,26,28,29,31,33,35,37,39-octadecaene tetrachloride (1:1) (9CI) (CA INDEX NAME)

CM 1

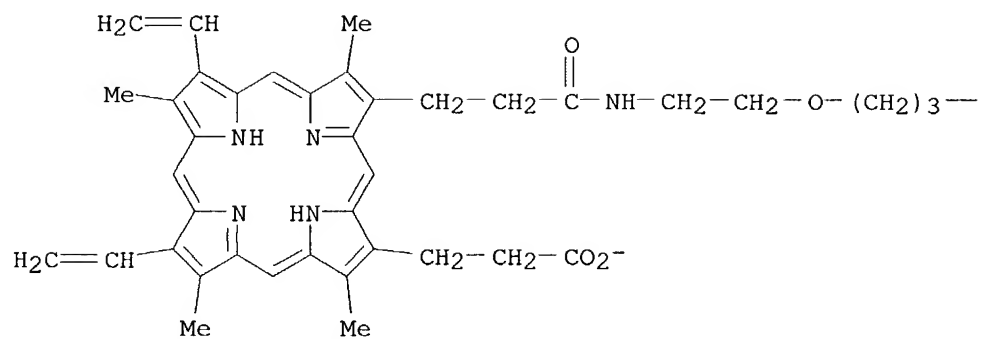
CRN 235438-51-4

CMF C96 H110 N11 O14 Ru . Cl H . Cl

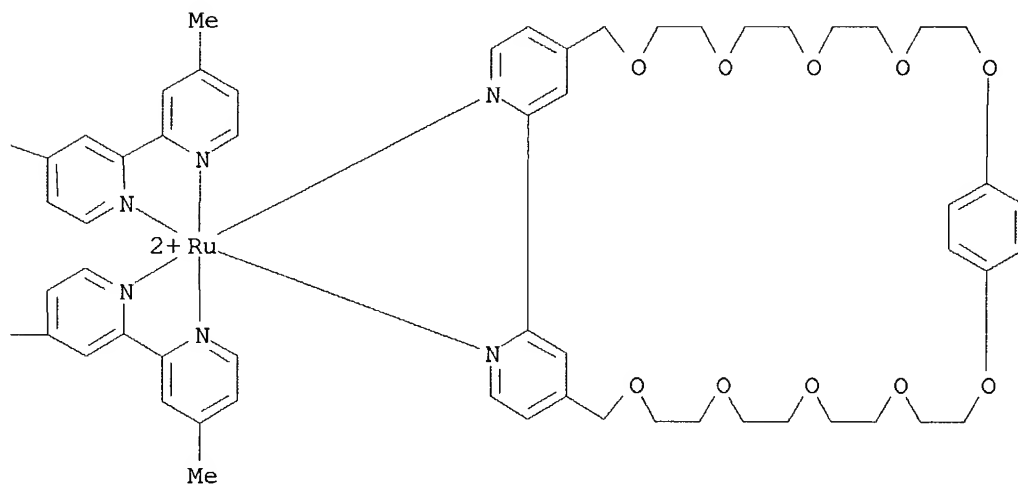
CCI CCS

PAGE 1-A

Me



PAGE 1-B



PAGE 2-A

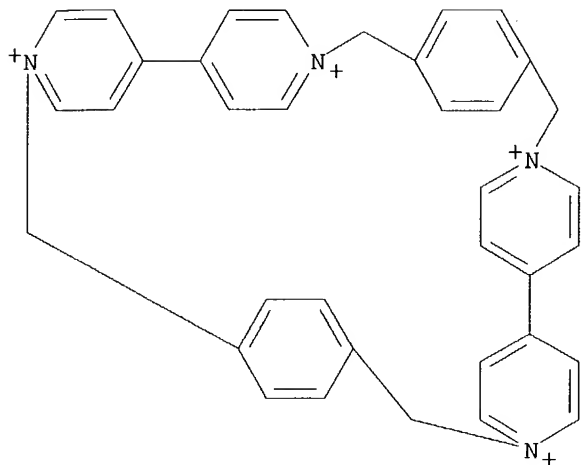
● Cl^-

● HCl

CM 2

CRN 117271-78-0

CMF C36 H32 N4 . 4 Cl



● 4 Cl⁻

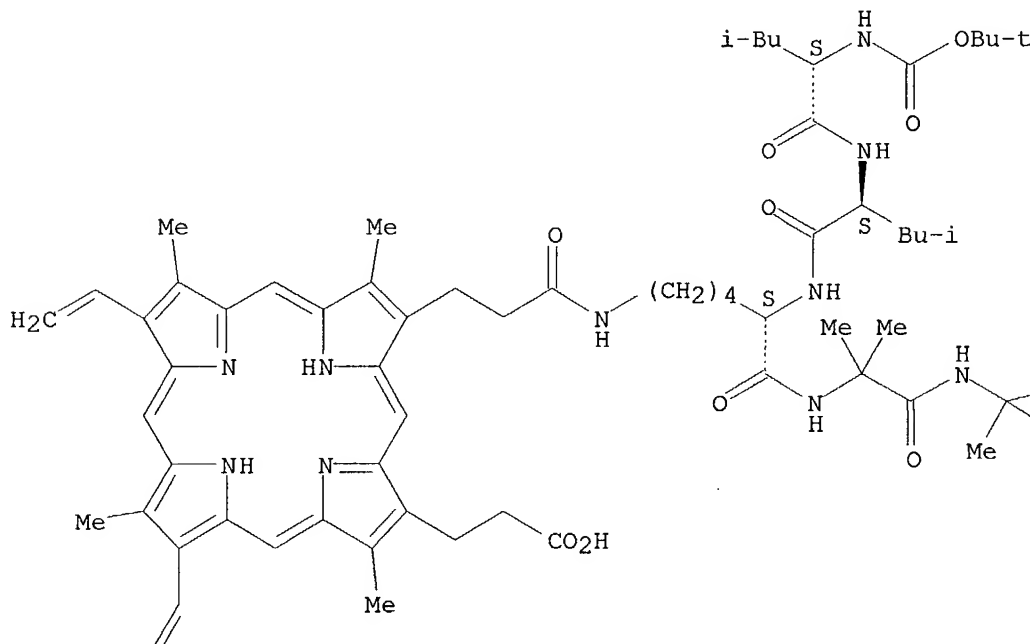
RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

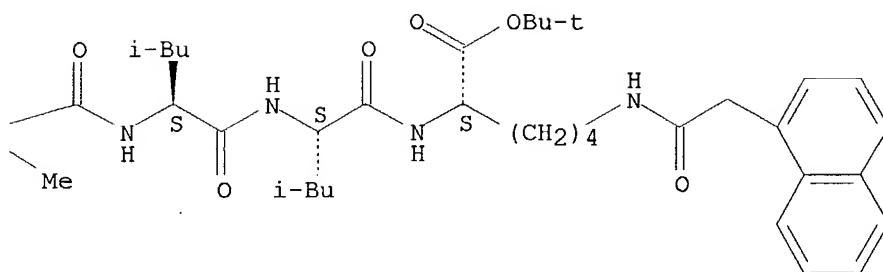
L7 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:528290 CAPLUS
DN 127:109178
TI Molecular Modeling of a Functionalized Aib-Based Octapeptide by Molecular
Mechanics Calculations Restrained by NMR and Fluorescence Data in DMSO
AU Pispisa, B.; Palleschi, A.; Amato, M. E.; Segre, A. L.; Venanzi, M.
CS Dipartimento di Scienze e Tecnologie Chimiche, Universita di Roma Tor
Vergata, Rome, 00133, Italy
SO Macromolecules (1997), 30(17), 4905-4910
CODEN: MAMOBX; ISSN: 0024-9297
PB American Chemical Society
DT Journal
LA English
AB The structural features of the sequential octapeptide Boc-(Leu)2-Lys(P)-
(Aib)2-(Leu)2-Lys(N)-OCMe₃, where P is protoporphyrin IX and N is
naphthalene, were investigated in DMSO by NMR and fluorescence
spectroscopy. Earlier IR, CD, and fluorescence results showed that this
compound attains a 310-helical conformation in methanol or water/methanol
(75/25, volume/volume). By contrast, the backbone structure in DMSO is
destroyed, but the high helix propensity of the Aib residues forces the
peptide to attain locally ordered arrangements, reminiscent of β -turn
features. Both NMR coupling constant and NOE connectivity data allowed the
computation of the structural features of part of the mol., but only their
combination with fluorescence results allowed the construction of the
whole mol. model. Implications of fluorescence data on the dynamics of
internal rotation of the chromophores are briefly discussed.

IT 171736-16-6
 RL: PRP (Properties)
 (conformation of aminoisobutyric acid peptide by by mol. mechanics
 calcns. restrained by NMR and fluorescence data in DMSO)
 RN 171736-16-6 CAPLUS
 CN L-Lysine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-L-leucyl-N6-[3-[18-(2-
 carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-
 oxopropyl]-L-lysyl-2-methylalanyl-2-methylalanyl-L-leucyl-L-leucyl-N6-(1-
 naphthalenylacetyl)-, 8-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

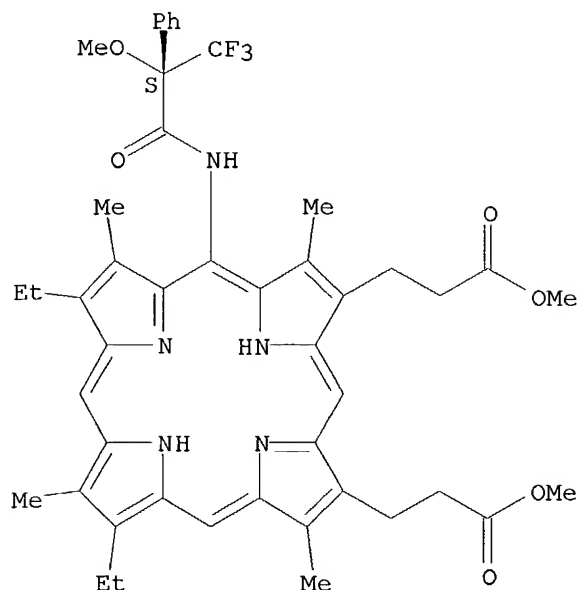
PAGE 1-A





L7 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1996:641877 CAPLUS
 DN 125:328358
 TI Synthesis, stereochemical and photophysical studies of chiral
 mesoporphyrins
 AU Poignant, Geraldine; Bourseul, Annie; Geze, Catherine; Plouzenec,
 Maryvonne Le; Le Maux, Paul; Bondon, Arnaud; Simonneaux, Gerard; Moinet,
 Claude; Vonarx, Veronique; Patrice, Thierry
 CS Lab. Chim. Organometallique Biol., CNRS, Rennes, 35042, Fr.
 SO Tetrahedron Letters (1996), 37(42), 7511-7514
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier
 DT Journal
 LA English
 AB The synthesis and NMR characterization of chiral mesoporphyrins bearing
 α -methoxy- α -(trifluoromethyl)phenylacetyl residues are
 reported. The phototoxicity with circular polarized light and
 intracellular localization in L1210 cells are also described as
 preliminary results.
 IT **183558-97-6P**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); BIOL (Biological
 study); PREP (Preparation)
 (synthesis, stereochem. and photophys. studies of chiral
 mesoporphyrins)
 RN 183558-97-6 CAPLUS
 CN 21H,23H-Porphine-2,18-dipropanoic acid, 8,13-diethyl-3,7,12,17-tetramethyl-
 5-[(3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl)amino]-, dimethyl
 ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1996:189170 CAPLUS
 DN 124:317836
 TI Conformational Statistics and Energetics Analysis of Sequential Peptides
 Undergoing Intramolecular Transfer of Excitation Energy
 AU Pispisa, B.; Palleschi, A.; Venanzi, M.; Zanotti, G.
 CS Dipartimento di Scienze e Tecnologie Chimiche, Universita di Roma Tor
 Vergata, Rome, 00133, Italy
 SO Journal of Physical Chemistry (1996), 100(16), 6835-44
 CODEN: JPCHAX; ISSN: 0022-3654
 PB American Chemical Society
 DT Journal
 LA English
 AB The photophysics of short linear peptides of general formula
 Boc-Leu-Leu-Lys(P)-(AA)_n-Leu-Leu-Lys(N)-OCMe₃ [AA = Ala, n = 1-4; AA =
 α-aminoisobutyric acid (Aib), n = 1-2; P = protoporphyrin IX, N =
 1-naphthylacetyl] were investigated in 75/25 (volume/volume) water/methanol by
 steady-state and time-resolved fluorescence expts. Quenching of the
 excited naphthyl chromophore takes place by electronic energy transfer to
 the porphyrin ground state, and proceeds on a time scale of 3-8 ns. A
 minor and slower fluorescence lifetime measures the decay of the
 exciplexes. Quenching efficiencies exhibit a different trend, depending
 on whether AA = Ala or Aib, indicating differences in the structural
 features of the two series of peptides. Consistently, CD spectra suggest
 that the former compds. populate α-helical structures, while the
 latter ones possibly attain a 310-helix conformation, in agreement with
 the proven ability of Aib to form 310-helices in solution. The increased
 percentage of intramol. H-bonds in the P(Aib)_nN as compared to the
 corresponding P(Ala)_nN peptides, as determined by IR spectra in dilute CD₃OD or
 CDCl₃ solution, confirms this conclusion. The fluorescence results were
 satisfactorily described by a dipole-dipole interaction mechanism,
 provided the mutual orientations of N and P groups are taken into account,

which implies that interconversion among conformational substrates of chromophore linkage is slow on the time scale of the transfer process. Conformational statistics anal. shows a rather wide interprobe separation distance distribution for each peptide, owing to the aliphatic portion of the side-chains carrying the chromophores, but theor. conformational anal. indicates that only a few energetically favored conformers are the major contributors to the energy transfer process.

IT **171736-14-4 171736-16-6**

RL: PRP (Properties)

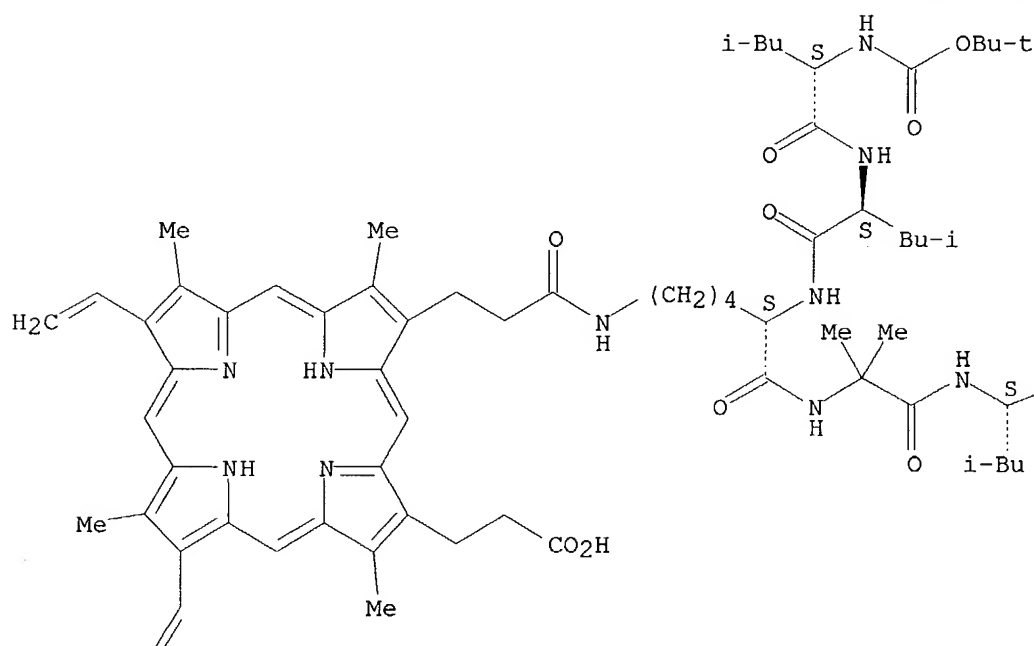
(conformational statistics and energetics anal. of sequential peptides undergoing intramol. transfer of excitation energy)

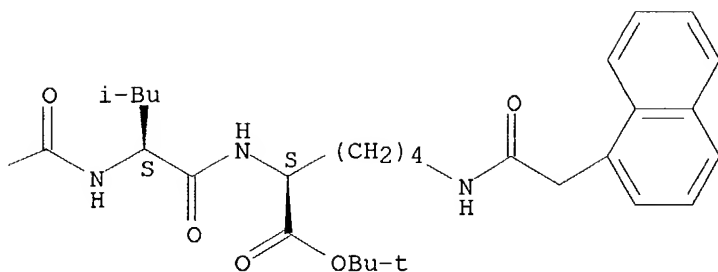
RN 171736-14-4 CAPLUS

CN L-Lysine, N2-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-2-methylalanyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

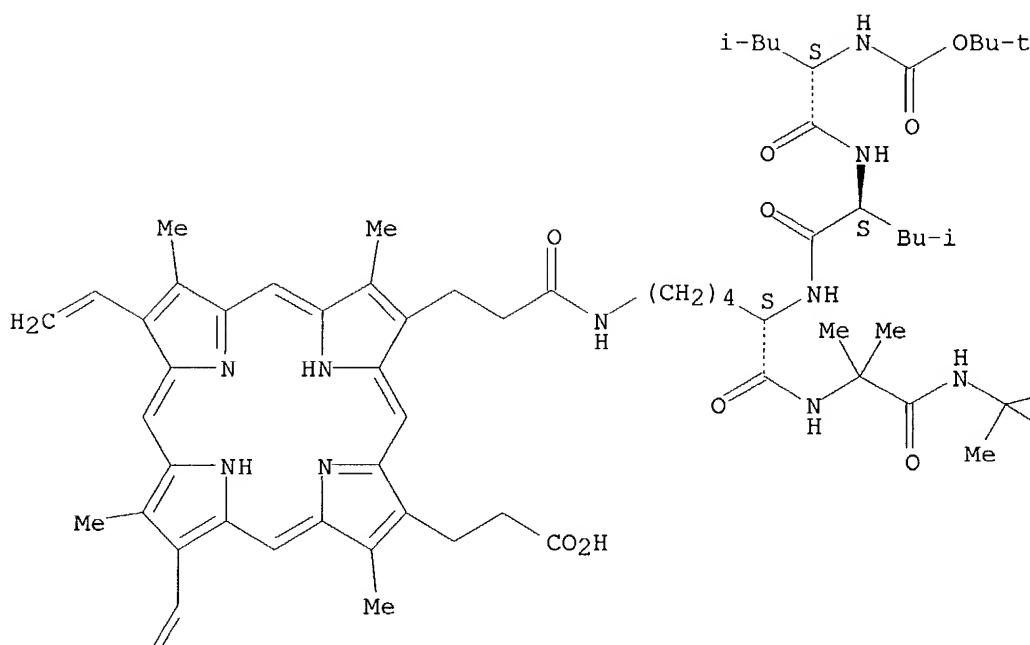




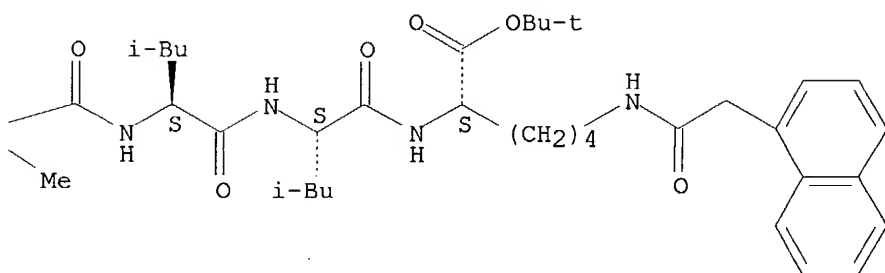
RN 171736-16-6 CAPLUS
 CN L-Lysine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-L-leucyl-N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-L-lysyl-2-methylalanyl-2-methylalanyl-L-leucyl-L-leucyl-N6-(1-naphthalenylacetyl)-, 8-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



PAGE 2-A



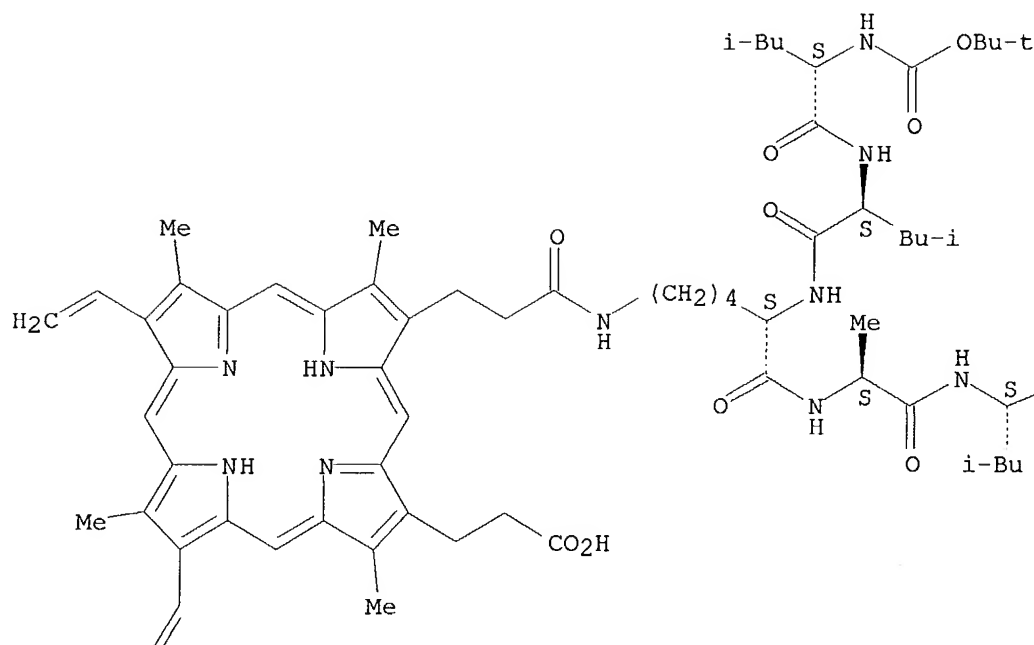
AN 1995:819429 CAPLUS
 DN 124:30371
 TI Intramolecular electronic energy transfer in peptides carrying naphthalene and protoporphyrin molecules: a spectroscopy and conformational statistics investigation
 AU Pispisa, B.; Venanzi, M.; Palleschi, A.; Zanotti, G.
 CS Dip. Science, Univ. Rome, Rome, 00133, Italy
 SO Biopolymers (1995), 36(4), 497-510
 CODEN: BIPMAA; ISSN: 0006-3525
 PB Wiley
 DT Journal
 LA English
 AB Short linear peptides, carrying an AA spacer in the backbone chain (AA = Aib or Ala) and naphthalene (N) and protoporphyrin IX (P) covalently bound to ϵ -amino groups of lysine side chains, were synthesized. The general formula is Boc-Leu-Leu-Lys(P)-(AA)_n-Leu-Leu-Lys(N)-OtBu (n = 0-2). The photophys. behavior of these compds. was investigated in water/methanol (75/25, volume/volume) solution by steady-state and time-resolved fluorescence expts. Quenching of excited naphthyl chromophore takes place by electronic energy transfer to the porphyrin ground state and proceeds on a time scale of 3-8 ns, while a minor and slower (\approx 45 ns) fluorescence lifetime measures the decay of the exciplexes. The results were compared with those obtained earlier for the P(Ala)_nN peptides (n = 0-4) in methanol solution, showing that addition of water does not significantly alter the dynamic relaxation behavior of the systems investigated, but affects the dissipation mechanism of the energy transferred to P. Quenching efficiencies from both fluorescence intensity and fluorescence lifetime measurement follow a different trend as the number of AA units increases, depending on whether AA = Aib or Ala, indicating that there are differences in the structural features of the two series of peptides. Consistently, CD spectral results suggest that the former compds. attain ordered conformations, possibly of the 3₁₀-helical type, while the latter populate α -helical structures to an extent depending on the chain length. Their IR data in dilute CD3OD or CDCl3 solution confirm this conclusion in that there is an increased percentage of intramol. H bonds in the P(Aib)_nN as compared to the corresponding P(Ala)_nN peptides. The photophys. results can be well described by a long-range dipole-dipole interaction model, provided the separation distances distribution and mutual orientation of N and P groups are taken into account. The need for using the angular relationships between the probes implies that interconversion among conformational substrates of chromophore linkages is slow on the time scale of the transfer process, very likely because of both the amide bond in the linkages and the bulkiness of the donor-acceptor pair.

IT **171736-17-7 171736-18-8 171736-19-9**
 RL: PRP (Properties)
 (intramol. electronic energy transfer in peptides carrying naphthalene and protoporphyrin mols. in relation to conformational anal.)

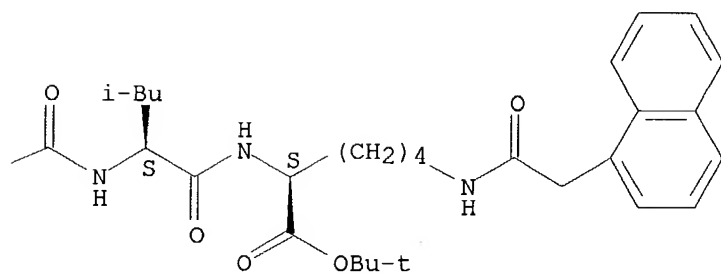
RN 171736-17-7 CAPLUS
 CN L-Lysine, N2-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-L-alanyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



PAGE 2-A

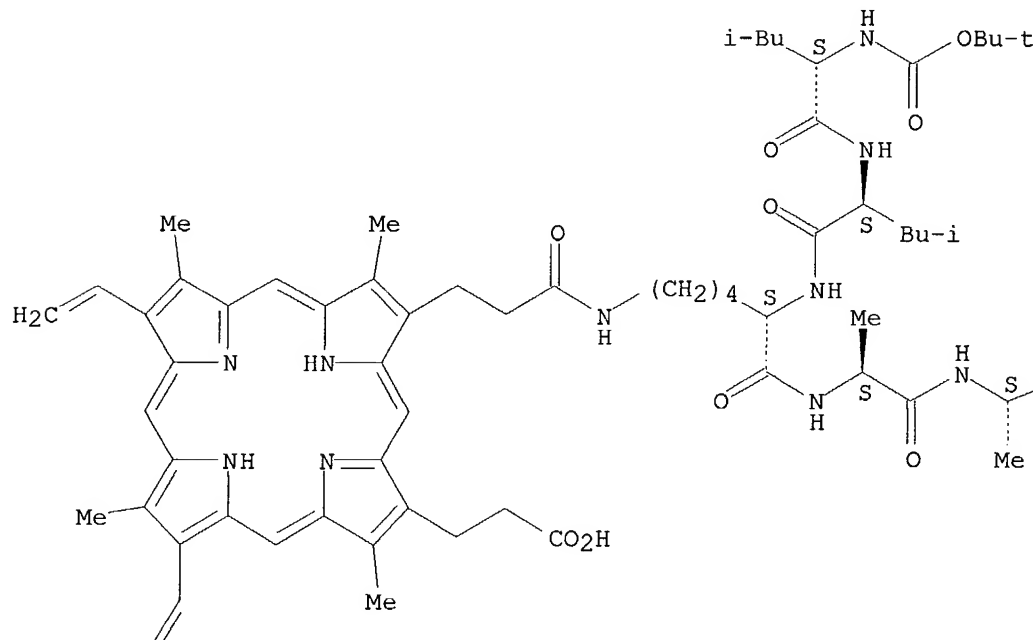


RN 171736-18-8 CAPLUS
 CN L-Lysine, N2-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[1,1-

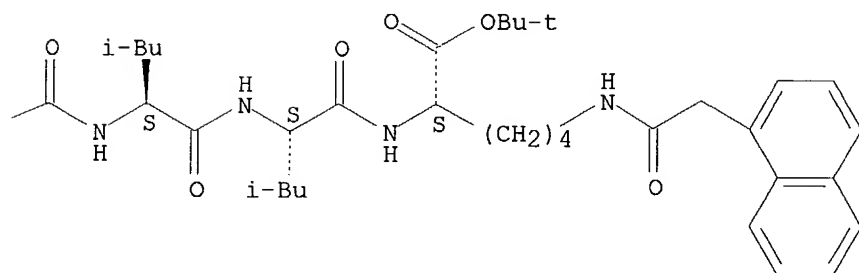
dimethylethoxy) carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-L-alanyl]-L-alanyl]-
L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl)
ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



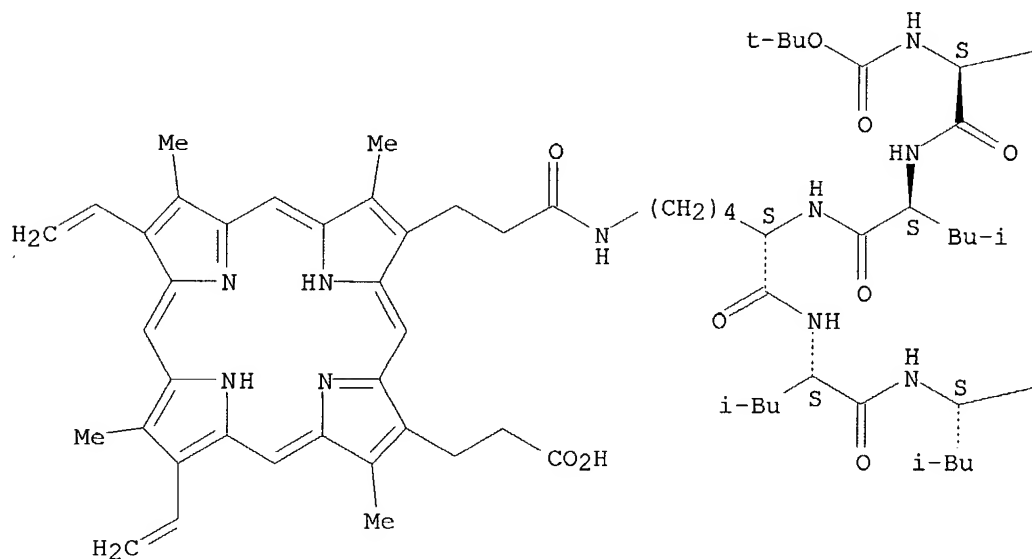
H₂C //

RN 171736-19-9 CAPLUS

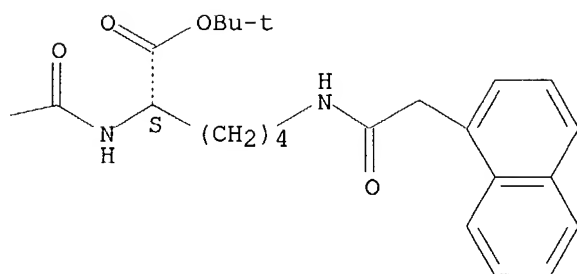
CN L-Lysine, N2-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



— Bu-i



IT 171736-14-4P 171736-16-6P

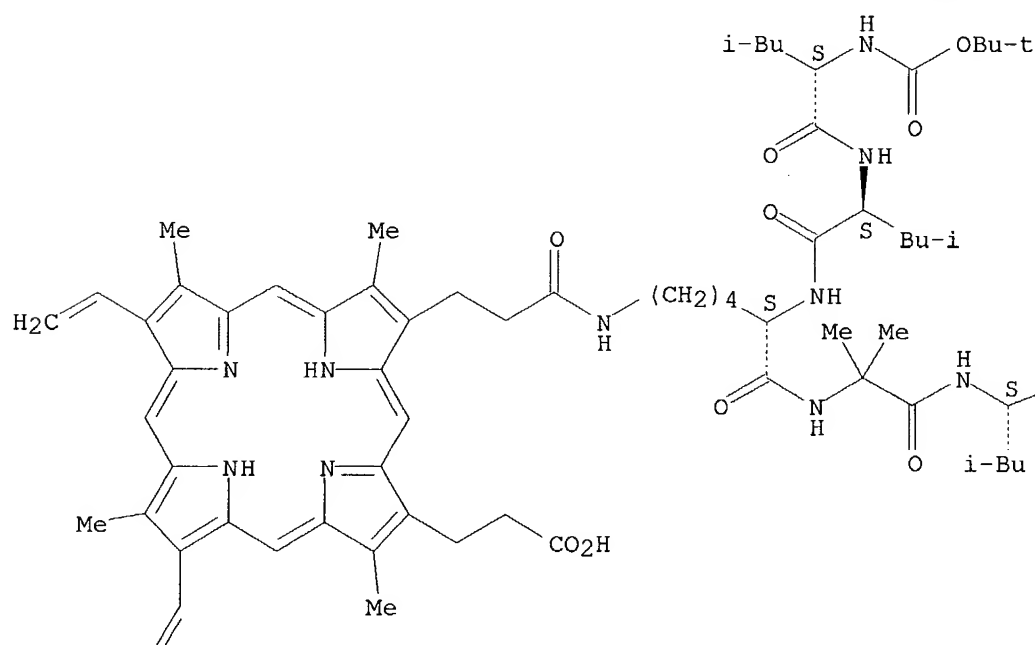
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (intramol. electronic energy transfer in peptides carrying naphthalene
 and protoporphyrin mols. in relation to conformational anal.)

RN 171736-14-4 CAPLUS

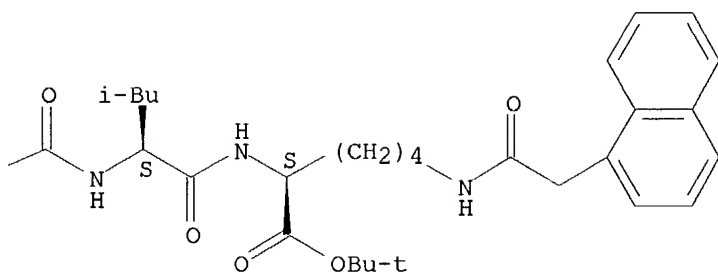
CN L-Lysine, N2-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-
 tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-
 dimethylethoxy) carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-2-methylalanyl]-L-
 leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



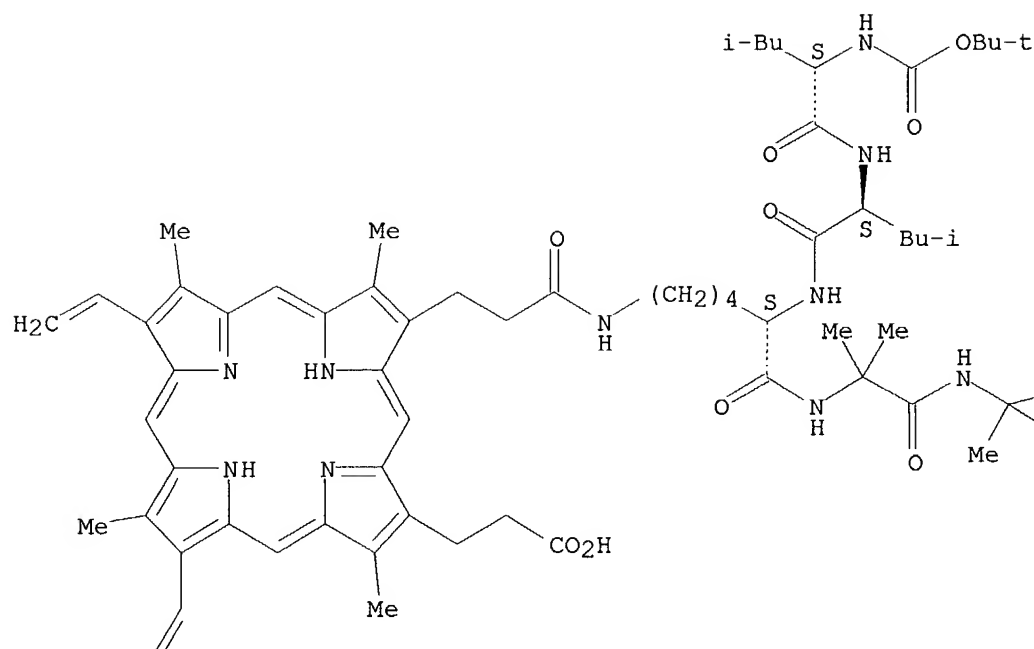
PAGE 2-A



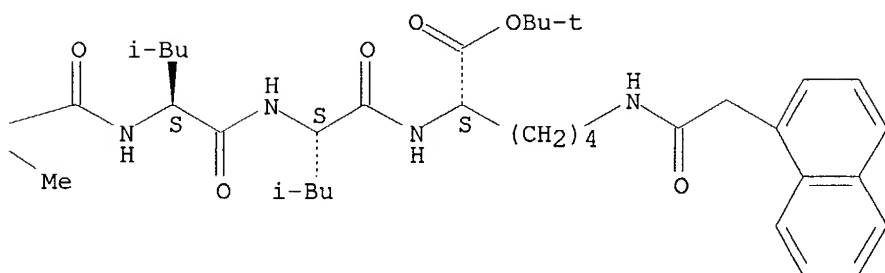
RN 171736-16-6 CAPLUS
CN L-Lysine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-L-leucyl-N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-L-lysyl-2-methylalanyl-2-methylalanyl-L-leucyl-L-leucyl-N6-(1-naphthalenylacetyl)-, 8-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



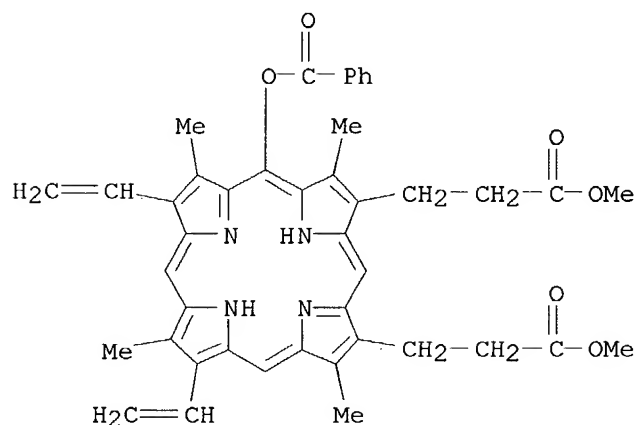
PAGE 1-B



PAGE 2-A



AN 1988:21587 CAPLUS
 DN 108:21587
 TI Synthetic and biosynthetic studies of porphyrins. Part 11. The synthesis of meso oxygenated protoporphyrins
 AU Jackson, Anthony H.; Rao, K. R. Nagaraja; Wilkins, Martyn
 CS Dep. Chem., Univ. Coll., Cardiff, CF1 1XL, UK
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (2), 307-12
 CODEN: JCPRB4; ISSN: 0300-922X
 DT Journal
 LA English
 OS CASREACT 108:21587
 AB Protoporphyrin IX di-Me ester (I; R-R3 = H) was treated with (BzO)₂ to give a mixture of 4 meso-benzoyloxy derivs. I (R = OBz, R1-R3 = H; R1 = OBz, R = R2 = R3 = H; R2 = OBz, R = R1 = R3 = H; R3 = OBz, R-R2 = H) (II). The mixture II was hydrolyzed to the corresponding oxyporphyrins, complexed with Fe, and oxidized with mol. O to give 4 biliverdin di-Me esters III. Conditions for the HPLC sepns. of II and III are discussed.
 IT **83807-58-3P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and basic hydrolysis of)
 RN 83807-58-3 CAPLUS
 CN 21H,23H-Porphine-2,18-dipropanoic acid, 5-(benzoyloxy)-8,13-diethenyl-3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



L7 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1986:202979 CAPLUS
 DN 104:202979
 TI On the mechanism of the chemical and enzymic oxygenations of α -oxyprotohemin IX to iron-biliverdin IX α
 AU Sano, Seiyo; Sano, Toyo; Morishima, Isao; Shiro, Yoshitugu; Maeda, Yutaka
 CS Dep. Public Health, Fac. Med., Kyoto, 606, Japan
 SO Proceedings of the National Academy of Sciences of the United States of America (1986), 83(3), 531-5
 CODEN: PNASA6; ISSN: 0027-8424
 DT Journal
 LA English
 AB α -Oxyprotohemin IX (I), an early intermediate in heme catabolism, was synthesized and its autoxidn. to biliverdin IX α was studied. In

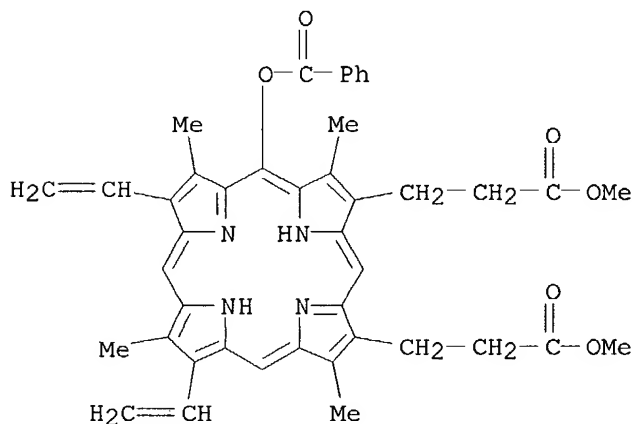
anaerobic aqueous pyridine, I (hexacoordinated) underwent autoxidn. to yield an Fe(II)-I π -neutral radical bis(pyridine) complex, which reacted with an equimolar amount of O₂ to give verdohemochrome IX α (II)-pyridine and CO in 75-80% yield via an intermediate with an absorption maximum at 893 nm. II did not react with further O₂. Reconstituted apomyoglobin-I complex (pentacoordinated) reacted with an equimolar amount of O₂ to form an Fe(II)-oxyporphyrin π -neutral radical intermediate, which rearranged to a green compound (λ_{max} 660 and 704 nm) with elision of CO. The green product, which is probably an apomyoglobin-verdoheme π -radical complex, reacted with another equimolar amount of O₂ to give Fe(III)-biliverdin IX α . Demetallation of this gave biliverdin IX α in an overall yield of 70-75%. Apparently, the 2-step sequence of oxyheme autoxidn. in the presence of apomyoglobin is α -oxyprotoheme IX \rightarrow II π -radical \rightarrow Fe(III)-biliverdin IX α (with CO leaving in the 1st step). A similar mechanism may prevail in vivo. the hexa- and pentacoordinated Fe(II) π -radical form of the oxyporphyrin is crucial in triggering the autoxidn. of the complex to verdohemochrome IX α . The hexa- and pentacoordinated Fe(II) π -radical form of the oxyporphyrin was crucial in triggering the autoxidn. of the complex to II. Further oxygenation of II to Fe(III)-biliverdin IX α occurred only in the pentacoordinated apomyoglobin-verdoheme Fe(II) complex.

IT 83807-58-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and deprotection of and iron insertion in)

RN 83807-58-3 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanoic acid, 5-(benzoyloxy)-8,13-diethenyl-3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



L7 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1983:45748 CAPLUS

DN 98:45748

TI Heminopeptide complexes which are models of an "active center" of oxygen-transferring hemoproteides. Synthesis and properties

AU Kazakova, N. A.; Radyukhin, V. A.; Luzgina, V. N.; Filippovich, E. I.; Kamysan, N. V.; Kudryavtseva, E. V.; Evstigneeva, R. P.

CS Mosk. Inst. Tonkoi Khim. Tekhnol., Moscow, USSR

SO Zhurnal Obshchei Khimii (1982), 52(8), 1896-906

CODEN: ZOKHA4; ISSN: 0044-460X

DT Journal

LA Russian

AB Unsym. 6(7), 7(6)-bis(amino acyl)peptide derivs. of protohemin IX (models of active centers of Hb and myoglobin) were prepared. The stability consts. were determined for the mono- and bis(amino acyl)peptide derivs. of protohemin IX with axial N-containing ligands (1-methylimidazole); the covalently-bound peptide has a stabilizing effect on the formation and stability of the 5-coordinate complexes. The hydrophobic spatial environment around the Fe ion of the ferroporphyrin 5-coordinate complexes affects their stability toward oxidation and their ability to coordinate CO at room temperature

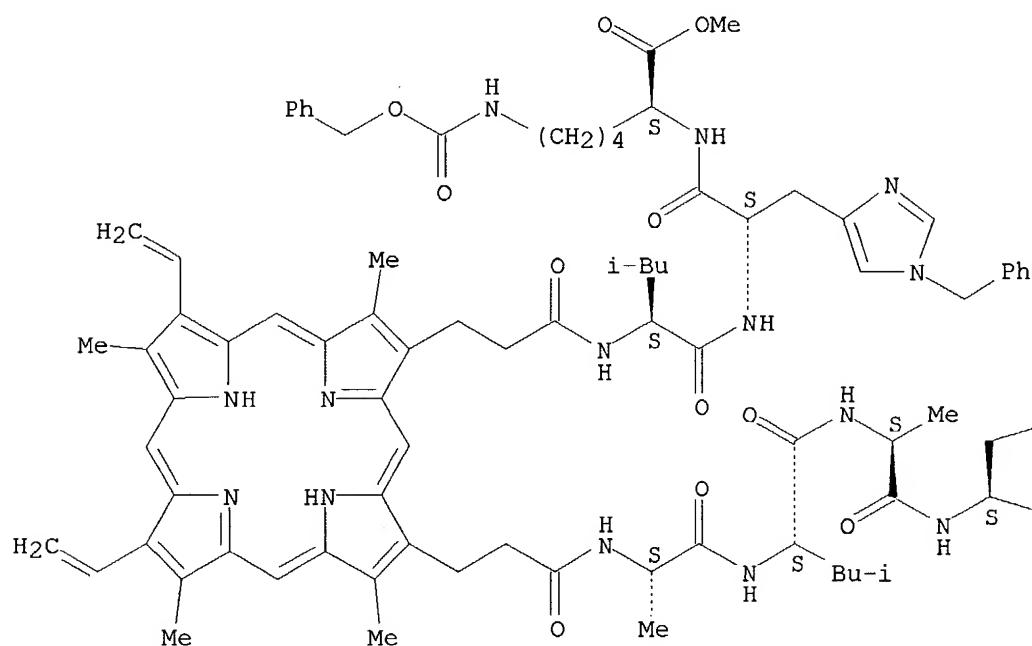
IT **83841-59-2D**, iron complexes with methylimidazole and pyridine
 RL: PRP (Properties)
 (stability consts. of)

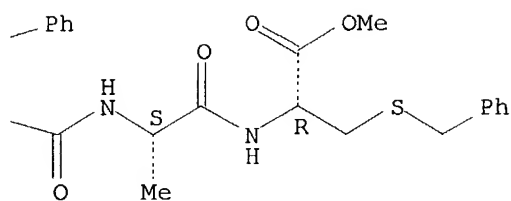
RN 83841-59-2 CAPLUS

CN L-Cysteine, N-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-L-alanyl-L-leucyl-L-alanyl-L-phenylalanyl-L-alanyl-S-(phenylmethyl)-, 6-methyl ester, (1→1')-amide with L-leucyl-1-(phenylmethyl)-L-histidyl-N6-[(phenylmethoxy)carbonyl]-L-lysine methyl ester (9CI) (CA INDEX NAME)

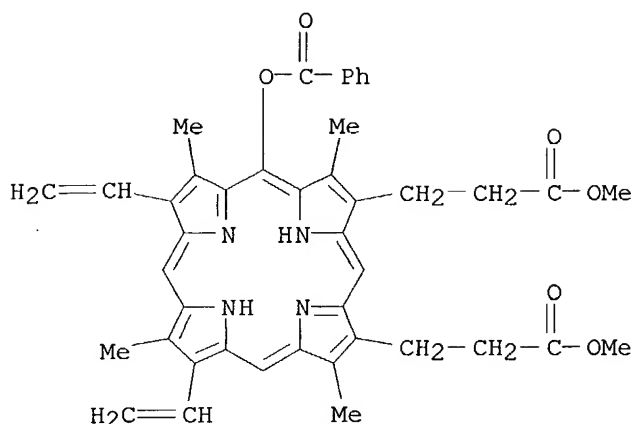
Absolute stereochemistry.

PAGE 1-A





L7 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1982:615860 CAPLUS
 DN 97:215860
 TI Synthesis of the four meso-oxyprotoporphyrin isomers
 AU Jackson, Anthony H.; Rao, K. R. Nagaraja; Wilkins, Martyn
 CS Dep. Chem., Univ. Coll., Cardiff, CF1 1XL, UK
 SO Journal of the Chemical Society, Chemical Communications (1982), (14),
 794-6
 CODEN: JCCCAT; ISSN: 0022-4936
 DT Journal
 LA English
 AB Oxidation of protoporphyrin IX di-Me ester with Bz2O2 in PhCl at 95°
 for 5 min gave a mixture of the 4 title compds. I (1 of R-R3 = OBz, other R
 groups = H) in 20% yield. I were separated by h.p.l.c. and identified by
 conversion to the corresponding biliverdins by passage in a 1:1 CHCl3/C6H6
 solution through a column of basic Al2O3, conversion to Fe complexes, and
 oxygenation in pyridine.
 IT **83807-58-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and conversion of, to corresponding biliverdin)
 RN 83807-58-3 CAPLUS
 CN 21H,23H-Porphine-2,18-dipropanoic acid, 5-(benzoyloxy)-8,13-diethenyl-
 3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



L7 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1980:621062 CAPLUS
 DN 93:221062
 TI Unsymmetrical 6,7-peptidylprotohemin IX
 IN Molokoedov, A. S.; Radyukhin, V. A.; Filippovich, E. I.; Evstigneeva, R. P.
 PA Moscow Institute of Fine Chemical Technology, USSR
 SO U.S.S.R.
 From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1980, (7), 117.
 CODEN: URXXAF

DT Patent
 LA Russian

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	SU 717039	T	19800225	SU 1978-2606603	19780331
				SU 1978-2606603	19780331

AB Title compds. I [R = PhCH₂O, Leu-His(CH₂Ph)-Lys(Z)-OMe (Z = PhCH₂O₂C), R₁ = Leu-His-Ala-Lys(Z)-Gly-Cys(CH₂Ph)-OCH₂Ph, Ala-Leu-Ala-Phe-Ala-Cys(CH₂Ph)-OCH₂Ph; R = Leu-His-Ala-Lys(Z)-Gly-Cys(CH₂Ph)-OCH₂Ph, Ala-Leu-Ala-Phe-Ala-Cys(CH₂Ph)-OCH₂Ph, R₁ = PhCH₂O, Leu-His(CH₂Ph)-Lys(Z)-OMe] were prepared by esterifying I (R = PhCH₂O, R₁ = HO; R = HO, R₁ = PhCH₂O) with C₆H₅OH by the mixed anhydride method with ClCO₂Et and condensing the resulting pentachlorophenyl active esters with the appropriate hexapeptides in 2.5-3 M urea solution at 40-45°.

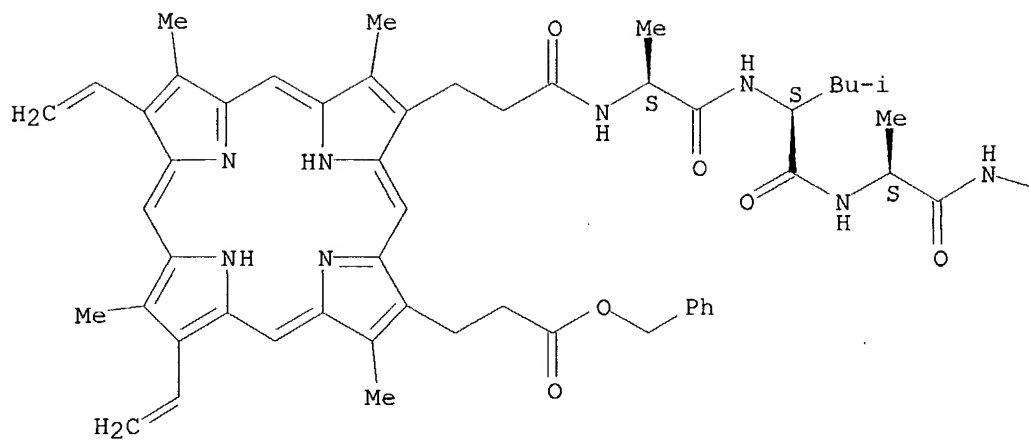
IT **75561-35-2DP**, complex with iron chloride
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 75561-35-2 CAPLUS

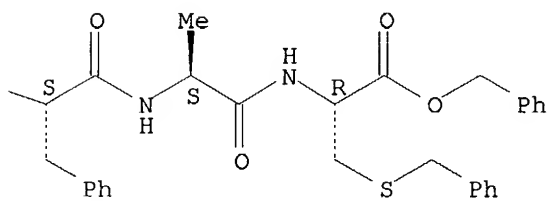
CN L-Cysteine, N-[N-[N-[N-[N-[3-[8,13-diethenyl-3,7,12,17-tetramethyl-18-[3-oxo-3-(phenylmethoxy)propyl]-21H,23H-porphin-2-yl]-1-oxopropyl]-L-alanyl]-L-leucyl]-L-alanyl]-L-phenylalanyl]-L-alanyl]-S-(phenylmethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

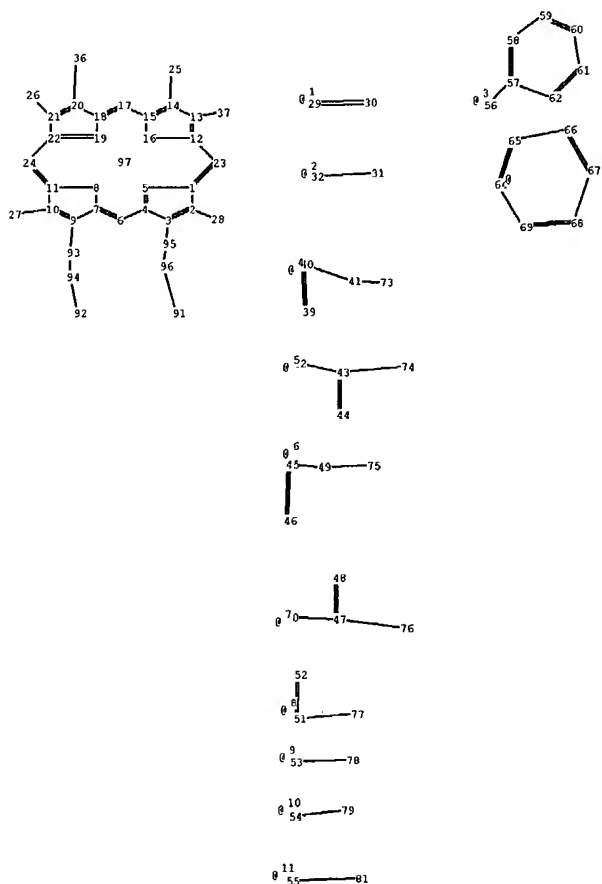
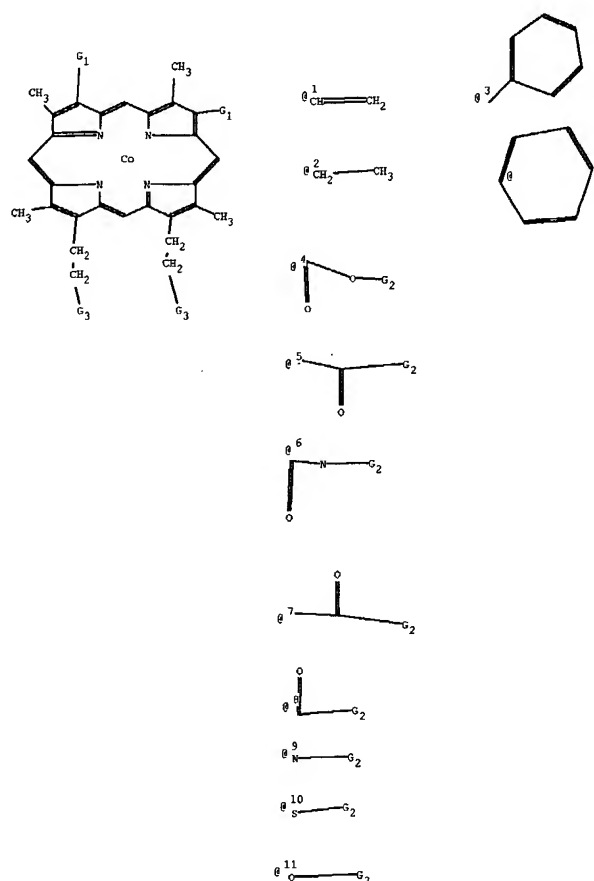
PAGE 1-A



PAGE 1-B



=>



chain nodes :

25 26 27 28 29 30 31 32 36 37 39 40 41 42 43 44 45 46
 47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
 91 92 93 94 95 96 97

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
 21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69

chain bonds :

2-28 3-95 9-93 10-27 13-37 14-25 20-36 21-26 29-30 31-32
 39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
 47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-96 92-94
 93-94 95-96

ring bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11
 11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19
 18-20 19-22 20-21 21-22 22-24 57-58 57-62 58-59 59-60 60-61
 61-62 64-65 64-69 65-66 66-67 67-68 68-69

exact/norm bonds :

7-8 8-11 12-16 13-37 15-16 20-36 39-40 40-41 41-73 42-43
 43-44 43-74 45-46 45-49 47-48 47-50 47-76 49-75 51-52 51-77
 53-78 54-79 55-81 91-96 92-94

exact bonds :

2-28 3-95 9-93 10-27 14-25 21-26 29-30 31-32 56-57 93-94
 95-96

normalized bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
 12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
 22-24 57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
 66-67

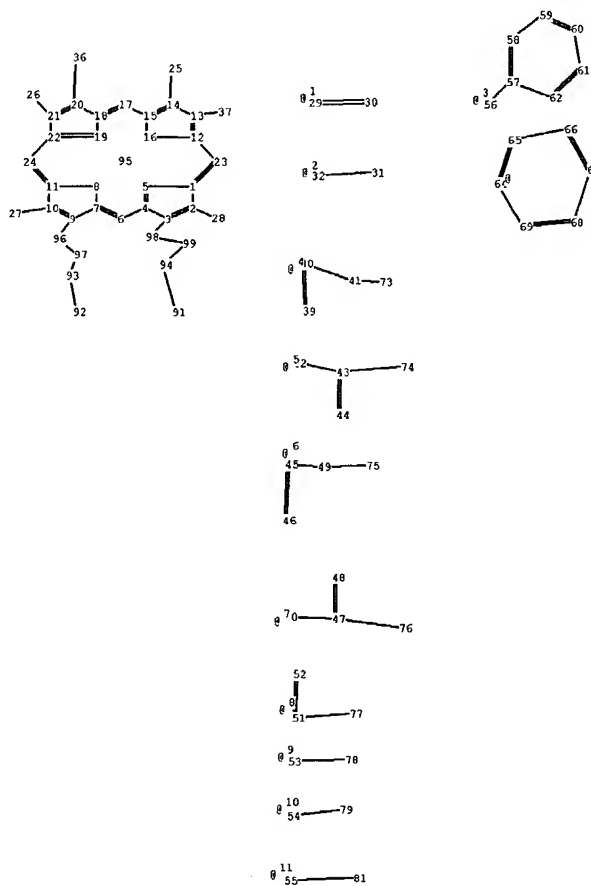
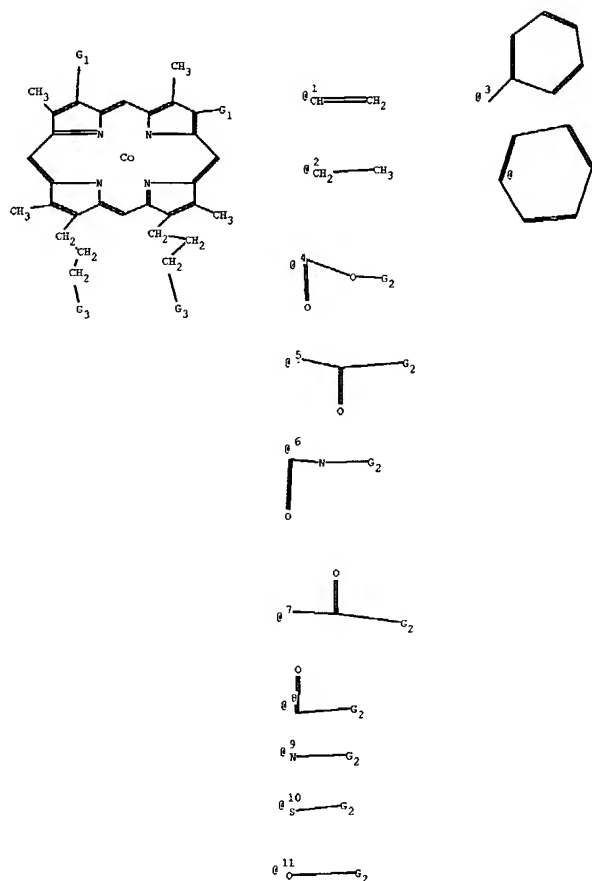
G1: [*1], [*2]

G2: H, CH₃, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*2], [*3]

G3: [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11]

Match level :

1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom
10:Atom	11:Atom	12:Atom	13:Atom	14:Atom	15:Atom	16:Atom	17:Atom	
18:Atom	19:Atom	20:Atom	21:Atom	22:Atom	23:Atom	24:Atom	25:Atom	
26:Atom	27:Atom	28:Atom	29:Atom	30:Atom	31:Atom	32:Atom	36:Atom	
37:Atom	39:CLASS	40:CLASS	41:Atom	42:Atom	43:Atom	44:Atom		
45:CLASS	46:CLASS	47:CLASS	48:CLASS	49:CLASS	50:CLASS	51:CLASS		
52:CLASS	53:CLASS	54:CLASS	55:CLASS	56:CLASS	57:Atom	58:Atom		
59:Atom	60:Atom	61:Atom	62:Atom	64:Atom	65:Atom	66:Atom	67:Atom	
68:Atom	69:Atom	73:CLASS	74:CLASS	75:CLASS	76:CLASS	77:CLASS		
78:CLASS	79:CLASS	81:CLASS	91:CLASS	92:CLASS	93:CLASS	94:CLASS		
95:CLASS	96:CLASS	97:CLASS						



chain nodes :

25 26 27 28 29 30 31 32 36 37 39 40 41 42 43 44 45 46
 47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
 91 92 93 94 95 96 97 98 99

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
 21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69

chain bonds :

2-28 3-98 9-96 10-27 13-37 14-25 20-36 21-26 29-30 31-32
 39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
 47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-94 92-93
 93-97 94-99 96-97 98-99

ring bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11
 11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19
 18-20 19-22 20-21 21-22 22-24 57-58 57-62 58-59 59-60 60-61
 61-62 64-65 64-69 65-66 66-67 67-68 68-69

exact/norm bonds :

7-8 8-11 12-16 13-37 15-16 20-36 39-40 40-41 41-73 42-43
 43-44 43-74 45-46 45-49 47-48 47-50 47-76 49-75 51-52 51-77
 53-78 54-79 55-81 91-94 92-93

exact bonds :

2-28 3-98 9-96 10-27 14-25 21-26 29-30 31-32 56-57 93-97
 94-99 96-97 98-99

normalized bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
 12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
 22-24 57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
 66-67

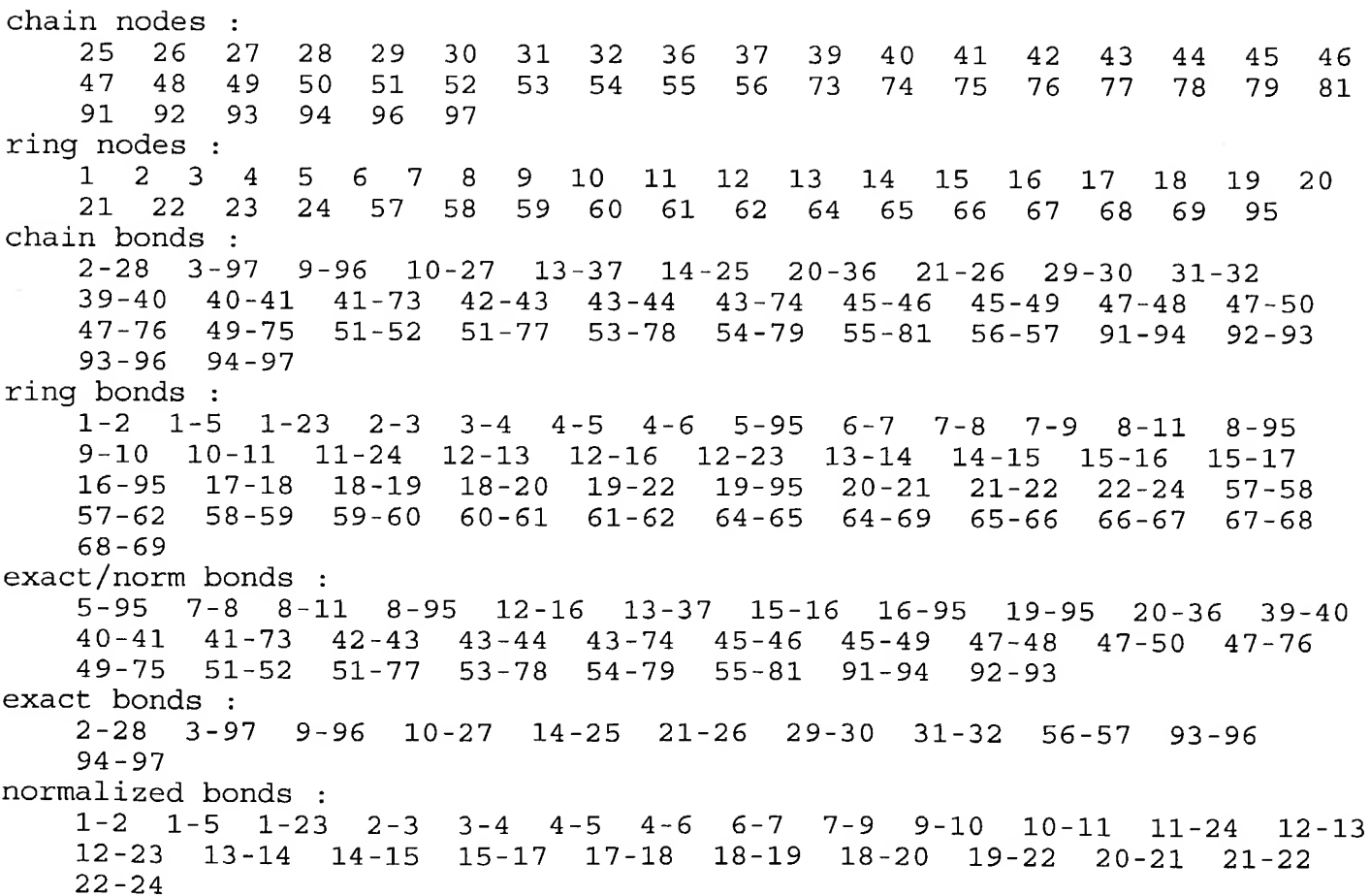
G1: [*1], [*2]

G2: H, CH₃, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*2], [*3]

G3: [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11]

Match level :

1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom
10:Atom	11:Atom	12:Atom	13:Atom	14:Atom	15:Atom	16:Atom	17:Atom	
18:Atom	19:Atom	20:Atom	21:Atom	22:Atom	23:Atom	24:Atom	25:Atom	
26:Atom	27:Atom	28:Atom	29:Atom	30:Atom	31:Atom	32:Atom	36:Atom	
37:Atom	39:CLASS	40:CLASS	41:Atom	42:Atom	43:Atom	44:Atom		
45:CLASS	46:CLASS	47:CLASS	48:CLASS	49:CLASS	50:CLASS	51:CLASS		
52:CLASS	53:CLASS	54:CLASS	55:CLASS	56:CLASS	57:Atom	58:Atom		
59:Atom	60:Atom	61:Atom	62:Atom	64:Atom	65:Atom	66:Atom	67:Atom	
68:Atom	69:Atom	73:CLASS	74:CLASS	75:CLASS	76:CLASS	77:CLASS		
78:CLASS	79:CLASS	81:CLASS	91:CLASS	92:CLASS	93:CLASS	94:CLASS		
95:CLASS	96:CLASS	97:CLASS	98:CLASS	99:CLASS				



57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
66-67 67-68 68-69

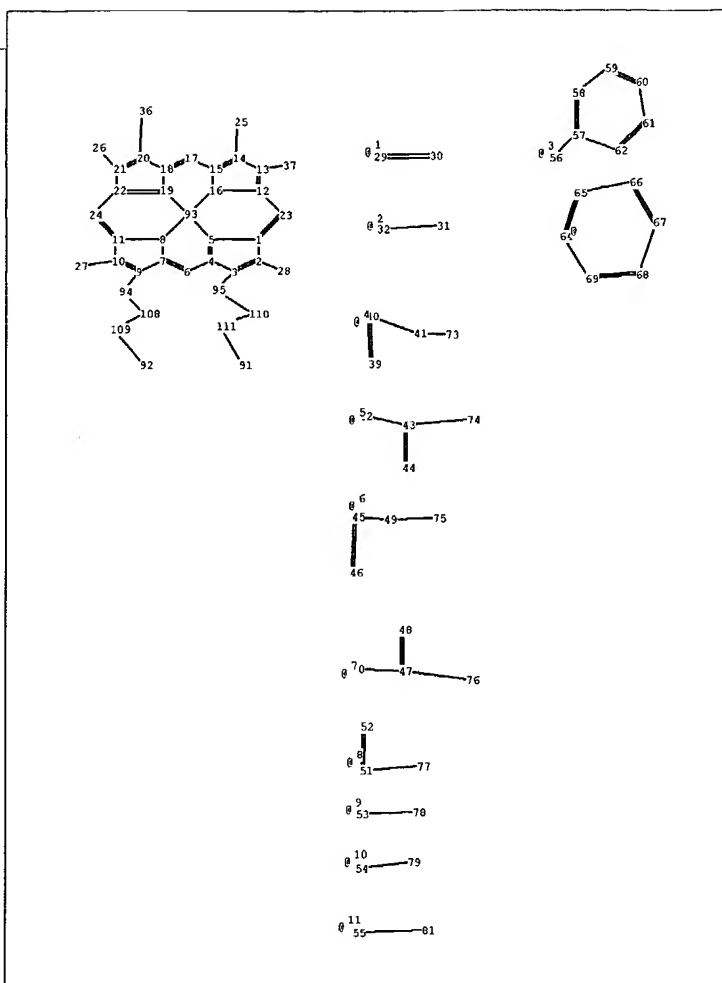
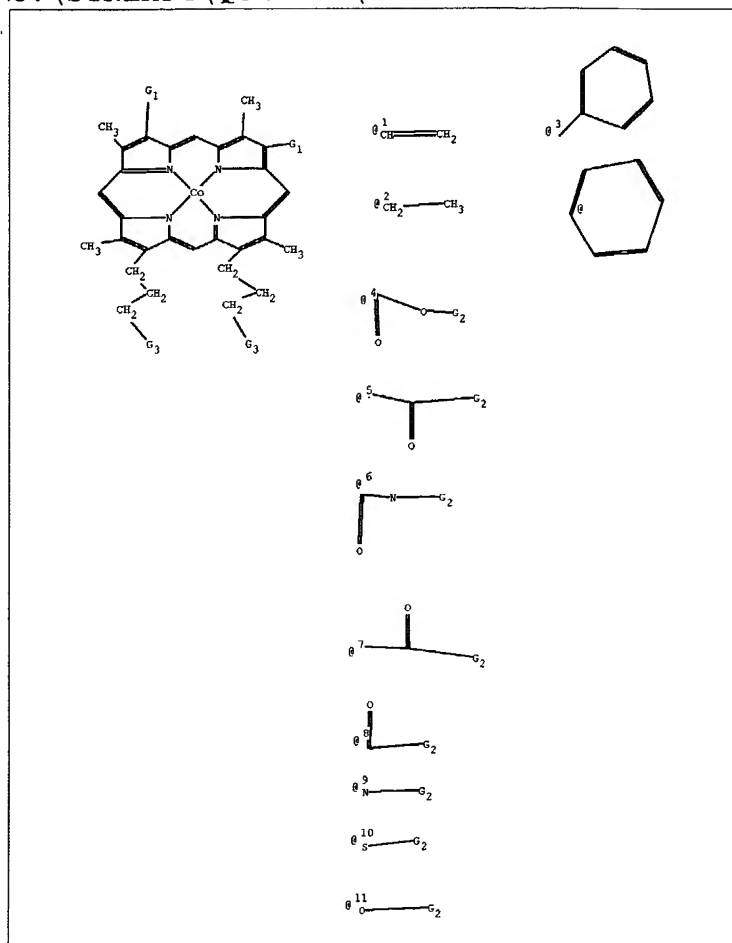
G1: [*1], [*2]

G2: H, CH3, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*2], [*3]

G3: [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 36:Atom
37:Atom 39:CLASS 40:CLASS 41:Atom 42:Atom 43:Atom 44:Atom
45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:Atom 58:Atom
59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom
68:Atom 69:Atom 73:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS
78:CLASS 79:CLASS 81:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS
95:CLASS 96:CLASS 97:CLASS



chain nodes :

25 26 27 28 29 30 31 32 36 37 39 40 41 42 43 44 45 46
 47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
 91 92 94 95 108 109 110 111

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
 21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69 93

chain bonds :

2-28 3-95 9-94 10-27 13-37 14-25 20-36 21-26 29-30 31-32
 39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
 47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-111 92-109
 94-108 95-110 108-109 110-111

ring bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 5-93 6-7 7-8 7-9 8-11 8-93
 9-10 10-11 11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17
 16-93 17-18 18-19 18-20 19-22 19-93 20-21 21-22 22-24 57-58
 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66 66-67 67-68
 68-69

exact/norm bonds :

5-93 7-8 8-11 8-93 12-16 13-37 15-16 16-93 19-93 20-36 39-40
 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50 47-76
 49-75 51-52 51-77 53-78 54-79 55-81 91-111 92-109

exact bonds :

2-28 3-95 9-94 10-27 14-25 21-26 29-30 31-32 56-57 94-108
 95-110 108-109 110-111

normalized bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13
 12-23 13-14 14-15 15-17 17-18 18-19 18-20 19-22 20-21 21-22
 22-24

57-58 57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66
66-67 67-68 68-69

G1:[*1],[*2]

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*2],[*3]

G3:[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 36:Atom
37:Atom 39:CLASS 40:CLASS 41:Atom 42:Atom 43:Atom 44:Atom
45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:Atom 58:Atom
59:Atom 60:Atom 61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom
68:Atom 69:Atom 73:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS
78:CLASS 79:CLASS 81:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS
95:CLASS 108:CLASS 109:CLASS 110:CLASS 111:CLASS

\$%^STN;HighlightOn= ***;HighlightOff=*** ;

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptaul29pxo

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS	4	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/CAPLUS
NEWS	5	FEB 05	German (DE) application and patent publication number format changes
NEWS	6	MAR 03	MEDLINE and LMEADLINE reloaded
NEWS	7	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	8	MAR 03	FRANCEPAT now available on STN
NEWS	9	MAR 29	Pharmaceutical Substances (PS) now available on STN
NEWS	10	MAR 29	WPIFV now available on STN
NEWS	11	MAR 29	No connect hour charges in WPIFV until May 1, 2004
NEWS	12	MAR 29	New monthly current-awareness alert (SDI) frequency in RAPRA
NEWS	13	APR 26	PROMT: New display field available
NEWS	14	APR 26	IFIPAT/IFIUDB/IFICDB: New super search and display field available
NEWS	15	APR 26	LITALERT now available on STN
NEWS	16	APR 27	NLDB: New search and display fields available
NEWS	EXPRESS		MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
NEWS	HOURS		STN Operating Hours Plus Help Desk Availability
NEWS	INTER		General Internet Information
NEWS	LOGIN		Welcome Banner and News Items
NEWS	PHONE		Direct Dial and Telecommunication Network Access to STN
NEWS	WWW		CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 14:24:50 ON 03 MAY 2004

=>

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY
7.35

SESSION
7.35

FILE 'REGISTRY' ENTERED AT 14:45:41 ON 03 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 30 APR 2004 HIGHEST RN 678535-01-8
DICTIONARY FILE UPDATES: 30 APR 2004 HIGHEST RN 678535-01-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>
Uploading C:\STNEXP4\QUERIES\867a.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 14:46:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 466 TO ITERATE

100.0% PROCESSED 466 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 8025 TO 10615
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> search l1
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 14:46:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 9800 TO ITERATE

100.0% PROCESSED 9800 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.01

L3 13 SEA SSS FUL L1

=>
Uploading C:\STNEXP4\QUERIES\867b.str

L4 STRUCTURE UPLOADED

=> d 14
L4 HAS NO ANSWERS
L4 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 14
SAMPLE SEARCH INITIATED 14:47:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 557 TO ITERATE

100.0% PROCESSED 557 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 9725 TO 12555
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> search 14
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 14:47:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 11654 TO ITERATE

100.0% PROCESSED 11654 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
 ENTRY SESSION
FULL ESTIMATED COST 311.68 319.03

FILE 'CAPLUS' ENTERED AT 14:48:01 ON 03 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 3 May 2004 VOL 140 ISS 19
FILE LAST UPDATED: 2 May 2004 (20040502/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L7 11 L3

=> d fbib ab hitstr 1-11

L7 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:721210 CAPLUS

DN 134:17340

TI Total synthesis and conformational analysis of monophenyl substituted protoporphyrins IX

AU Robinsohn, Adriana E.; Maier, Marta S.; Buldain, Graciela Y.

CS Facultad de Farmacia y Bioquimica, Universidad de Buenos Aires, Buenos Aires, 1113, Argent.

SO Heterocycles (2000), 53(10), 2127-2142

CODEN: HTCYAM; ISSN: 0385-5414

PB Japan Institute of Heterocyclic Chemistry

DT Journal

LA English

OS CASREACT 134:17340

AB The total synthesis of meso-monoaryl protoporphyrins [I; R1 = Ph, R2R3 = (II)] and [I; R1R3 = H, R2 = Ph (III)] using a MacDonald type [2+2] condensation is described. In this method a bisformyl dipyrromethane is treated with a biscarboxydipyrromethane. Attempts to obtain the .delta.-meso-monoaryl protoporphyrin [I; R1R2 = H, R3 = Ph (IV)] by the a,c-biladiene method failed as it could not be prepd. starting from its tripyrrrene precursor (V). The synthesis of the V is described. Mol. modeling studies allowed us to find the most favorable conformations for II and III. In both porphyrins, the exocyclic Ph group adopts a noncoplanar disposition relative to the plane of the macrocycle. In porphyrin III the macrocycle is nearly planar while nonplanar saddle conformation was obtained for porphyrin II.

IT ***309757-24-2P***

RL: PNU (Preparation, unclassified); PREP (Preparation)
(attempted prepn. of)

RN 309757-24-2 CAPLUS

CN 21H,23H-Porphine-2,18-dipropionic acid, 8,13-diethenyl-3,7,12,17-tetramethyl-5-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)

/ Structure 1 in file .gra /

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1999:367089 CAPLUS

DN 131:110291

TI A convenient synthesis of a Ru(bpy)3-based catenane-type triad and its incorporation into a protein scaffold

AU Hu, Yi-Zhen; Tsukiji, Shinya; Shinkai, Seiji; Hamachi, Itaru

CS Department of Chemistry and Biochemistry, Graduate School of Engineering, Kyushu University, Fukuoka, 812-8581, Japan

SO Chemistry Letters (1999), (6), 517-518

CODEN: CMLTAG; ISSN: 0366-7022

PB Chemical Society of Japan

DT Journal

LA English

AB A catenated heme cofactor consisting of a sensitizer (Ru(bpy)2L (L = I)), a donor (protoheme) II (R = 4'-methyl-2,2'-bipyridin-4-yl) and an accepto

(cyclobis(paraquat-p-phenylene) (III)) was prepd. by stepwise coordination, followed by Fe-insertion. Reconstitution of apomyoglobin with this cofactor afforded a protein-based, noncovalently-linked photosynthetic triad.

IT

231302-74-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reactant for prepn. of iron porphyrinate ruthenium bipyridine bipryidinocrown ether catenated with cyclobisparaquatphenylene for incorporation in protein scaffold)

RN

231302-74-2 CAPLUS

CN

Ruthenium(1+), (2,5,8,11,14,27,30,33,36,39-decaoxa-19,22-diazatetracyclo[38.2.2.116,20.121,25]hexatetraconta-16,18,20(46),21,23,25(45),40,42,43-nonaene-.kappa.N19,.kappa.N22)[8,13-diethenyl-3,7,12,17-tetramethyl-18-[3-[[2-[3-(4'-methyl[2,2'-bipyridin]-4-yl-.kappa.N1,.kappa.N1')propoxy]ethyl]amino]-3-oxopropyl]-21H,23H-porphin 2-propanoato(1-)](4,4'-dimethyl-2,2'-bipyridine-.kappa.N1,.kappa.N1')-, (OC-6-43)-, chloride, monohydrochloride, catena compd. with 5,12,19,26-tetraazoniaheptacyclo[24.2.2.22,5.27,10.212,15.216,19.221,24]t traconta-2,4,7,9,12,14,16,18,21,23,26,28,29,31,33,35,37,39-octadecaene tetrachloride (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 235438-51-4

CMF C96 H110 N11 O14 Ru . Cl H . Cl

CCI CCS

/ Structure 2 in file .gra /

/ Structure 3 in file .gra /

/ Structure 4 in file .gra /

CM 2

CRN 117271-78-0

CMF C36 H32 N4 . 4 Cl

/ Structure 5 in file .gra /

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:528290 CAPLUS

DN 127:109178

TI Molecular Modeling of a Functionalized Aib-Based Octapeptide by Molecular Mechanics Calculations Restrained by NMR and Fluorescence Data in DMSO

AU Pispisa, B.; Palleschi, A.; Amato, M. E.; Segre, A. L.; Venanzi, M.

CS Dipartimento di Scienze e Tecnologie Chimiche, Universita di Roma Tor Vergata, Rome, 00133, Italy

SO Macromolecules (1997), 30(17), 4905-4910

CODEN: MAMOBX; ISSN: 0024-9297

PB American Chemical Society

DT Journal

LA English
AB The structural features of the sequential octapeptide Boc-(Leu)2-Lys(P)-(Aib)2-(Leu)2-Lys(N)-OCMe3, where P is protoporphyrin IX and N is naphthalene, were investigated in DMSO by NMR and fluorescence spectroscopy. Earlier IR, CD, and fluorescence results showed that this compd. attains a 310-helical conformation in methanol or water/methanol (75/25, vol./vol.). By contrast, the backbone structure in DMSO is destroyed, but the high helix propensity of the Aib residues forces the peptide to attain locally ordered arrangements, reminiscent of .beta.-turn features. Both NMR coupling const. and NOE connectivity data allowed the computation of the structural features of part of the mol., but only their combination with fluorescence results allowed the construction of the whole mol. model. Implications of fluorescence data on the dynamics of internal rotation of the chromophores are briefly discussed.

IT ***171736-16-6***

RL: PRP (Properties)

(conformation of aminoisobutyric acid peptide by by mol. mechanics
calcns. restrained by NMR and fluorescence data in DMSO)

RN 171736-16-6 CAPLUS

CN L-Lysine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-L-leucyl-N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-oxopropyl]-L-lysyl-2-methylalanyl-2-methylalanyl-L-leucyl-L-leucyl-N6-(1-naphthalenylacetyl)-, 8-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 6 in file .gra /

/ Structure 7 in file .gra /

/ Structure 8 in file .gra /

L7 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1996:641877 CAPLUS

DN 125:328358

TI Synthesis, stereochemical and photophysical studies of chiral mesoporphyrins

AU Poignant, Geraldine; Bourseul, Annie; Geze, Catherine; Plouzenec, Maryvonne Le; Le Maux, Paul; Bondon, Arnaud; Simonneaux, Gerard; Moinet, Claude; Vonarx, Veronique; Patrice, Thierry

CS Lab. Chim. Organometallique Biol., CNRS, Rennes, 35042, Fr.

SO Tetrahedron Letters (1996), 37(42), 7511-7514

CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier

DT Journal

LA English

AB The synthesis and NMR characterization of chiral mesoporphyrins bearing .alpha.-methoxy-.alpha.-(trifluoromethyl)phenylacetyl residues are reported. The phototoxicity with circular polarized light and intracellular localization in L1210 cells are also described as preliminary results.

IT ***183558-97-6P***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis, stereochem. and photophys. studies of chiral mesoporphyrins)

RN 183558-97-6 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanoic acid, 8,13-diethyl-3,7,12,17-tetramethyl-5-[(3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl)amino]-, dimethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 9 in file .gra /

L7 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1996:189170 CAPLUS

DN 124:317836

TI Conformational Statistics and Energetics Analysis of Sequential Peptides Undergoing Intramolecular Transfer of Excitation Energy

AU Pispisa, B.; Palleschi, A.; Venanzi, M.; Zanutti, G.

CS Dipartimento di Scienze e Tecnologie Chimiche, Universita di Roma Tor Vergata, Rome, 00133, Italy

SO Journal of Physical Chemistry (1996), 100(16), 6835-44

CODEN: JPCHAX; ISSN: 0022-3654

PB American Chemical Society

DT Journal

LA English

AB The photophysics of short linear peptides of general formula Boc-Leu-Leu-Lys(P)-(AA)n-Leu-Leu-Lys(N)-OCMe₃ [AA = Ala, n = 1-4; AA = .alpha.-aminoisobutyric acid (Aib), n = 1-2; P = protoporphyrin IX, N = 1-naphthylacetyl] were investigated in 75/25 (vol./vol.) water/methanol by steady-state and time-resolved fluorescence expts. Quenching of the excited naphthyl chromophore takes place by electronic energy transfer to the porphyrin ground state, and proceeds on a time scale of 3-8 ns. A minor and slower fluorescence lifetime measures the decay of the exciplexes. Quenching efficiencies exhibit a different trend, depending on whether AA = Ala or Aib, indicating differences in the structural features of the two series of peptides. Consistently, CD spectra suggest that the former compds. populate .alpha.-helical structures, while the latter ones possibly attain a 310-helix conformation, in agreement with the proven ability of Aib to form 310-helices in soln. The increased percentage of intramol. H-bonds in the P(Aib)_nN as compared to the corresponding P(Ala)_nN peptides, as detd. by IR spectra in dil. CD₃OD or CDCl₃ soln., confirms this conclusion. The fluorescence results were satisfactorily described by a dipole-dipole interaction mechanism, provided the mutual orientations of N and P groups are taken into account which implies that interconversion among conformational substrates of chromophore linkage is slow on the time scale of the transfer process. Conformational statistics anal. shows a rather wide interprobe sepn. distance distribution for each peptide, owing to the aliph. portion of the side-chains carrying the chromophores, but theor. conformational anal. indicates that only a few energetically favored conformers are the major contributors to the energy transfer process.

IT ***171736-14-4*** ***171736-16-6***

RL: PRP (Properties)

(conformational statistics and energetics anal. of sequential peptides undergoing intramol. transfer of excitation energy)

RN 171736-14-4 CAPLUS

CN L-Lysine, N2-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,1-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-2-methylalanyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 10 in file .gra /

/ Structure 11 in file .gra /

/ Structure 12 in file .gra /

RN 171736-16-6 CAPLUS
CN L-Lysine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-L-leucyl-N6-[3-[18-(2
carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-
oxopropyl]-L-lysyl-2-methylalanyl-2-methylalanyl-L-leucyl-L-leucyl-N6-(1-
naphthalenylacetyl)-, 8-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 13 in file .gra /

/ Structure 14 in file .gra /

/ Structure 15 in file .gra /

L7 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:819429 CAPLUS
DN 124:30371
TI Intramolecular electronic energy transfer in peptides carrying naphthalen
and protoporphyrin molecules: a spectroscopy and conformational statistic
investigation
AU Pispisa, B.; Venanzi, M.; Palleschi, A.; Zanotti, G.
CS Dip. Science, Univ. Rome, Rome, 00133, Italy
SO Biopolymers (1995), 36(4), 497-510
CODEN: BIPMAA; ISSN: 0006-3525
PB Wiley
DT Journal
LA English
AB Short linear peptides, carrying an AA spacer in the backbone chain (AA =
Aib or Ala) and naphthalene (N) and protoporphyrin IX (P) covalently boun
to .epsilon.-amino groups of lysine side chains, were synthesized. The
general formula is Boc-Leu-Leu-Lys(P)-(AA)n-Leu-Leu-Lys(N)-OtBu (n = 0-2)
The photophys. behavior of these compds. was investigated in
water/methanol (75/25, vol./vol.) soln. by steady-state and time-resolved
fluorescence expts. Quenching of excited naphthyl chromophore takes plac
by electronic energy transfer to the porphyrin ground state and proceeds
on a time scale of 3-8 ns, while a minor and slower (.apprxeq.45 ns)
fluorescence lifetime measures the decay of the exciplexes. The results
were compared with those obtained earlier for the P(Ala)nN peptides (n =
0-4) in methanol soln., showing that addn. of water does not significantl
alter the dynamic relaxation behavior of the systems investigated, but
affects the dissipation mechanism of the energy transferred to P.
Quenching efficiencies from both fluorescence intensity and fluorescence
lifetime measurement follow a different trend as the no. of AA units
increases, depending on whether AA = Aib or Ala, indicating that there ar
differences in the structural features of the two series of peptides.
Consistently, CD spectral results suggest that the former compds. attain
ordered conformations, possibly of the 310-helical type, while the latter
populate .alpha.-helical structures to an extent depending on the chain
length. Their IR data in dil. CD3OD or CDCl3 soln. confirm this
conclusion in that there is an increased percentage of intramol. H bonds

in the P(Aib)nN as compared to the corresponding P(Ala)nN peptides. The photophys. results can be well described by a long-range dipole-dipole interaction model, provided the sepn. distances distribution and mutual orientation of N and P groups are taken into account. The need for using the angular relationships between the probes implies that interconversion among conformational substrates of chromophore linkages is slow on the time scale of the transfer process, very likely because of both the amide bond in the linkages and the bulkiness of the donor-acceptor pair.

IT ***171736-17-7*** ***171736-18-8*** ***171736-19-9***
RL: PRP (Properties)
(intramol. electronic energy transfer in peptides carrying naphthalene and protoporphyrin mols. in relation to conformational anal.)
RN 171736-17-7 CAPLUS
CN L-Lysine, N2-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,1-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-L-alanyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

/ Structure 16 in file .gra /

/ Structure 17 in file .gra /

/ Structure 18 in file .gra /

RN 171736-18-8 CAPLUS
CN L-Lysine, N2-[N-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-L-alanyl]-L-alanyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 19 in file .gra /

/ Structure 20 in file .gra /

/ Structure 21 in file .gra /

RN 171736-19-9 CAPLUS
CN L-Lysine, N2-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 22 in file .gra /

/ Structure 23 in file .gra /

IT ***171736-14-4P*** ***171736-16-6P***
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (intramol. electronic energy transfer in peptides carrying naphthalene
 and protoporphyrin mols. in relation to conformational anal.)
RN 171736-14-4 CAPLUS
CN L-Lysine, N2-[N-[N-[N-[N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-N2-[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl]-L-leucyl]-L-lysyl]-2-methylalanyl]-L-leucyl]-L-leucyl]-N6-(1-naphthalenylacetyl)-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 24 in file .gra /

/ Structure 25 in file .gra /

/ Structure 26 in file .gra /

RN 171736-16-6 CAPLUS
CN L-Lysine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-L-leucyl-N6-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-L-lysyl-2-methylalanyl-2-methylalanyl-L-leucyl-L-leucyl-N6-(1-naphthalenylacetyl)-, 8-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 27 in file .gra /

/ Structure 28 in file .gra /

/ Structure 29 in file .gra /

L7 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1988:21587 CAPLUS
DN 108:21587
TI Synthetic and biosynthetic studies of porphyrins. Part 11. The synthesis of meso oxygenated protoporphyrins
AU Jackson, Anthony H.; Rao, K. R. Nagaraja; Wilkins, Martyn
CS Dep. Chem., Univ. Coll., Cardiff, CF1 1XL, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (2), 307-12
 CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
OS CASREACT 108:21587
AB Protoporphyrin IX di-Me ester (I; R-R3 = H) was treated with (BzO)₂ to give a mixt. of 4 meso-benzoyloxy derivs. I (R = OBz, R1-R3 = H; R1 = OBz, R = R2 = R3 = H; R2 = OBz, R = R1 = R3 = H; R3 = OBz, R-R2 = H) (II). The mixt. II was hydrolyzed to the corresponding oxyporphyrins, complexed with Fe, and oxidized with mol. O to give 4 biliverdin di-Me esters III.

Conditions for the HPLC sepns. of II and III are discussed.
IT ***83807-58-3P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and basic hydrolysis of)
RN 83807-58-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 5-(benzoyloxy)-8,13-diethenyl-
3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)

/ Structure 30 in file .gra /

L7 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:202979 CAPLUS
DN 104:202979
TI On the mechanism of the chemical and enzymic oxygenations of
.alpha.-oxyprotohemin IX to iron.cntdot.biliverdin IX.alpha.
AU Sano, Seiyo; Sano, Toyo; Morishima, Isao; Shiro, Yoshitugu; Maeda, Yutaka
CS Dep. Public Health, Fac. Med., Kyoto, 606, Japan
SO Proceedings of the National Academy of Sciences of the United States of
America (1986), 83(3), 531-5
CODEN: PNASA6; ISSN: 0027-8424
DT Journal
LA English
AB .alpha.-Oxyprotohemin IX (I), an early intermediate in heme catabolism,
was synthesized and its autoxidn. to biliverdin IX.alpha. was studied. I
anaerobic aq. pyridine, I (hexacoordinated) underwent autoredn. to yield
an Fe(II)-I .pi.-neutral radical bis(pyridine) complex, which reacted wit
an equimolar amt. of O2 to give verdohemochrome IX.alpha. (II)-pyridine
and CO in 75-80% yield via an intermediate with an absorption max. at 893
nm. II did not react with further O2. Reconstituted apomyoglobin-I
complex (pentacoordinated) reacted with an equimolar amt. of O2 to form a
Fe(II)-oxyporphyrin .pi.-neutral radical intermediate, which rearranged t
a green compd. (.lambda.max 660 and 704 nm) with elision of CO. The gree
product, which is probably an apomyoglobin-verdoheme .pi.-radical complex
reacted with another equimolar amt. of O2 to give Fe(III)-biliverdin
IX.alpha.. Demetallation of this gave biliverdin IX.alpha. in an overall
yield of 70-75%. Apparently, the 2-step sequence of oxyheme autoxidn. in
the presence of apomyoglobin is .alpha.-oxyprotoheme IX .fwdarw. II
.pi.-radical .fwdarw. Fe(III)-biliverdin IX.alpha. (with CO leaving in th
1st step). A similar mechanism may prevail in vivo.the hexa- and
pentacoordinated Fe(II) .pi.-radical form of the oxyporphyrin is crucial
in triggering the autoxidn. of the complex to verdohemochrome IX.alpha..
The hexa- and pentacoordinated Fe(II) .pi.-radical form of the
oxyporphyrin was crucial in triggering the autoxidn. of the complex to II
Further oxygenation of II to Fe(III)-biliverdin IX.alpha. occurred only i
the pentacoordinated apomyoglobin-verdoheme Fe(II) complex.

IT ***83807-58-3P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deprotection of and iron insertion in)
RN 83807-58-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 5-(benzoyloxy)-8,13-diethenyl-
3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)

/ Structure 31 in file .gra /

L7 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:45748 CAPLUS
DN 98:45748
TI Heminopeptide complexes which are models of an "active center" of

oxygen-transferring hemoproteides. Synthesis and properties
AU Kazakova, N. A.; Radyukhin, V. A.; Luzgina, V. N.; Filippovich, E. I.;
Kamyshan, N. V.; Kudryavtseva, E. V.; Evstigneeva, R. P.
CS Mosk. Inst. Tonkoi Khim. Tekhnol., Moscow, USSR
SO Zhurnal Obshchei Khimii (1982), 52(8), 1896-906
CODEN: ZOKHA4; ISSN: 0044-460X
DT Journal
LA Russian
AB Unsym. 6(7), 7(6)-bis(amino acyl)peptide derivs. of protohemin IX (models
of active centers of Hb and myoglobin) were prepd. The stability consts.
were detd. for the mono- and bis(amino acyl)peptide derivs. of protohemin
IX with axial N-contg. ligands (1-methylimidazole); the covalently-bound
peptide has a stabilizing effect on the formation and stability of the
5-coordinate complexes. The hydrophobic spatial environment around the F
ion of the ferroporphyrin 5-coordinate complexes affects their stability
toward oxidn. and their ability to coordinate CO at room temp.
IT ***83841-59-2D*** , iron complexes with methylimidazole and pyridine
RL: PRP (Properties)
(stability consts. of)
RN 83841-59-2 CAPLUS
CN L-Cysteine, N-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-
21H,23H-porphin-2-yl]-1-oxopropyl]-L-alanyl-L-leucyl-L-alanyl-L-
phenylalanyl-L-alanyl-S-(phenylmethyl)-, 6-methyl ester,
(1.fwdarw.1')-amide with L-leucyl-1-(phenylmethyl)-L-histidyl-N6-
[(phenylmethoxy)carbonyl]-L-lysine methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 32 in file .gra /

/ Structure 33 in file .gra /

L7 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:615860 CAPLUS
DN 97:215860
TI Synthesis of the four meso-oxyprotoporphyrin isomers
AU Jackson, Anthony H.; Rao, K. R. Nagaraja; Wilkins, Martyn
CS Dep. Chem., Univ. Coll., Cardiff, CF1 1XL, UK
SO Journal of the Chemical Society, Chemical Communications (1982), (14),
794-6
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
AB Oxidn. of protoporphyrin IX di-Me ester with Bz2O2 in PhCl at 95.degree.
for 5 min gave a mixt. of the 4 title compds. I (1 of R-R3 = OBz, other R
groups = H) in 20% yield. I were sepd. by h.p.l.c. and identified by
conversion to the corresponding biliverdins by passage in a 1:1 CHCl3/C6H
soln. through a column of basic Al2O3, conversion to Fe complexes, and
oxygenation in pyridine.
IT ***83807-58-3P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to corresponding biliverdin)
RN 83807-58-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropionic acid, 5-(benzoyloxy)-8,13-diethenyl-
3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)

/ Structure 34 in file .gra /

L7 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1980:621062 CAPLUS
 DN 93:221062
 TI Unsymmetrical 6,7-peptidylprotohemin IX
 IN Molokoedov, A. S.; Radyukhin, V. A.; Filippovich, E. I.; Evstigneeva, R.
 P.
 PA Moscow Institute of Fine Chemical Technology, USSR
 SO U.S.S.R.
 From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1980, (7), 117.
 CODEN: URXXAF
 DT Patent
 LA Russian
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	SU 717039	T	19800225	SU 1978-2606603	19780331
				SU 1978-2606603	19780331
AB	Title compds. I [R = PhCH ₂ O, Leu-His(CH ₂ Ph)-Lys(Z)-OMe (Z = PhCH ₂ O ₂ C), R ₁ = Leu-His-Ala-Lys(Z)-Gly-Cys(CH ₂ Ph)-OCH ₂ Ph, Ala-Leu-Ala-Phe-Ala-Cys(CH ₂ Ph)-OCH ₂ Ph; R = Leu-His-Ala-Lys(Z)-Gly-Cys(CH ₂ Ph)-OCH ₂ Ph, Ala-Leu-Ala-Phe-Ala-Cys(CH ₂ Ph)-OCH ₂ Ph, R ₁ = PhCH ₂ O, Leu-His(CH ₂ Ph)-Lys(Z)-OMe] were prepd. by esterifying I (R = PhCH ₂ O, R ₁ = HO; R = HO, R ₁ = PhCH ₂ O) with C ₆ H ₅ OH by the mixed anhydride method with ClCO ₂ Et and condensing the resulting pentachlorophenyl active esters with the appropriate hexapeptides in 2.5-M urea soln. at 40-45.degree..				
IT	***75561-35-2DP***, complex with iron chloride RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)				
RN	75561-35-2 CAPLUS				
CN	L-Cysteine, N-[N-[N-[N-[N-[3-[8,13-diethenyl-3,7,12,17-tetramethyl-18-[3-oxo-3-(phenylmethoxy)propyl]-21H,23H-porphin-2-yl]-1-oxopropyl]-L-alanyl]-L-leucyl]-L-alanyl]-L-phenylalanyl]-L-alanyl]-S-(phenylmethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)				

Absolute stereochemistry.

/ Structure 35 in file .gra /

/ Structure 36 in file .gra /

=>
 Uploading C:\STNEXP4\QUERIES\867c.str

L8 STRUCTURE UPLOADED

=>
 Uploading C:\STNEXP4\QUERIES\867d.str

L9 STRUCTURE UPLOADED

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
59.77	378.80

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION

FILE 'REGISTRY' ENTERED AT 14:57:55 ON 03 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 30 APR 2004 HIGHEST RN 678535-01-8
DICTIONARY FILE UPDATES: 30 APR 2004 HIGHEST RN 678535-01-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> s l8

SAMPLE SEARCH INITIATED 14:57:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 21 TO ITERATE

100.0% PROCESSED 21 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 146 TO 694
PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L8

=> search l8

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 14:58:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 363 TO ITERATE

100.0% PROCESSED 363 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L11 0 SEA SSS FUL L8

=> s l9

SAMPLE SEARCH INITIATED 14:58:16 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 22 TO ITERATE

100.0% PROCESSED 22 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 159 TO 721
PROJECTED ANSWERS: 0 TO 0

L12 0 SEA SSS SAM L9

=> search l9
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 14:58:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 421 TO ITERATE

100.0% PROCESSED 421 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L13 0 SEA SSS FUL L9

=>
Uploading C:\STNEXP4\QUERIES\867e.str

L14 STRUCTURE UPLOADED

=> s l14
SAMPLE SEARCH INITIATED 15:00:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 22 TO ITERATE

100.0% PROCESSED 22 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 159 TO 721
PROJECTED ANSWERS: 0 TO 0

L15 0 SEA SSS SAM L14

=> search l14
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 15:00:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 421 TO ITERATE

100.0% PROCESSED 421 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L16 0 SEA SSS FUL L14

=>
Uploading C:\STNEXP4\QUERIES\867f.str

L17 STRUCTURE UPLOADED

=> s l17
SAMPLE SEARCH INITIATED 15:01:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 21 TO ITERATE

100.0% PROCESSED 21 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 146 TO 694
PROJECTED ANSWERS: 0 TO 0

L18 0 SEA SSS SAM L17

=> search l17
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.

ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 15:01:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 363 TO ITERATE

100.0% PROCESSED 363 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

L19 2 SEA SSS FUL L17

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	623.36	1002.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-7.62

FILE 'CAPLUS' ENTERED AT 15:02:53 ON 03 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 3 May 2004 VOL 140 ISS 19
FILE LAST UPDATED: 2 May 2004 (20040502/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l19

L20 1 L19

=> d l19 fbib ab hitstr

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

=> d l20 fbib ab hitstr

L20 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:607121 CAPLUS
DN 97:207121
TI Synthesis of mono-S-aminoacyl derivatives of cobalt-porphyrin complexes containing peptides
AU Kazakova, N. A.; Nguyen Huy Doan; Filippovich, E. I.; Evstigneeva, R. P.
CS USSR
SO Deposited Doc. (1980), SPSTL 287khp-D80, 13 pp. Avail.: SPSTL
DT Report
LA Russian
AB I (R = CH₂:CH, H, COMe; R₁ = R₂ = OH) were converted to I (R = CH₂:CH, H, COMe; R₁ = LeuHisOMe, LeuHisAlaLysGlyCys(CH₂Ph)OCH₂Ph, LeuHisAlaPheAlaGlyOMe, R₂ = OH or vice versa). The peptide-contg. Co

porphyrins were characterized by IR spectra and electronic spectra. These complexes are easily oxidized in air and are reduced by Na₂S₂O₆ as indicated by electronic spectral data.

IT ***83118-03-0P*** ***83139-86-0P***

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 83118-03-0 CAPLUS

CN Cobaltate(1-), [1-methyl-N-[N-[N-[N-[N-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-L-leucyl]-L-histidyl]-L-alanyl]-L-phenylalanyl]-L-alanyl]glycinato(3-)-N21,N22,N23,N24]-, hydrogen, (SP-4-2)-(9CI) (CA INDEX NAME)

/ Structure 37 in file .gra /

/ Structure 38 in file .gra /

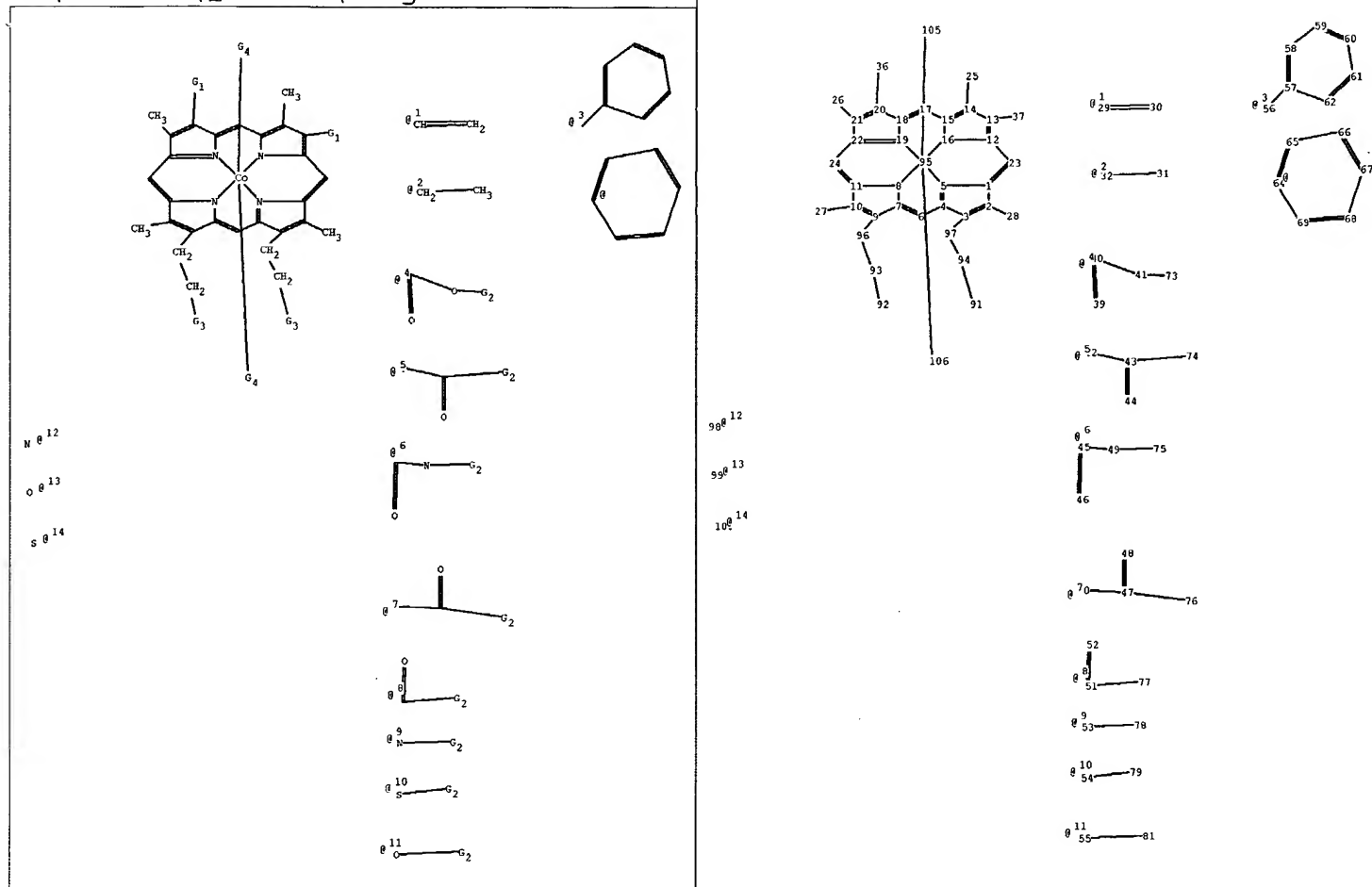
RN 83139-86-0 CAPLUS

CN Cobaltate(1-), [1-(phenylmethyl) N-[N-[N2-[N-[N-[N-[3-[18-(2-carboxyethyl)-8,13-diethenyl-3,7,12,17-tetramethyl-21H,23H-porphin-2-yl]-1-oxopropyl]-L-leucyl]-L-histidyl]-L-alanyl]-N6-[(phenylmethoxy) carbonyl]-L-lysyl]glycyl S-(phenylmethyl)-L-cysteinato(3-)-N21,N22,N23,N24]-, hydrogen, (SP-4-2)-(9CI) (CA INDEX NAME)

/ Structure 39 in file .gra /

/ Structure 40 in file .gra /

=>



chain nodes :

25	26	27	28	29	30	31	32	36	37	39	40	41	42	43	44	45	46
47	48	49	50	51	52	53	54	55	56	73	74	75	76	77	78	79	81
91	92	93	94	96	97	105	106										

ring nodes :

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
21	22	23	24	57	58	59	60	61	62	64	65	66	67	68	69	95			

ring/chain nodes :

98	99	100
----	----	-----

chain bonds :

2-28	3-97	9-96	10-27	13-37	14-25	20-36	21-26	29-30	31-32
39-40	40-41	41-73	42-43	43-44	43-74	45-46	45-49	47-48	47-50
47-76	49-75	51-52	51-77	53-78	54-79	55-81	56-57	91-94	92-93
93-96	94-97	95-105	95-106						

ring bonds :

1-2	1-5	1-23	2-3	3-4	4-5	4-6	5-95	6-7	7-8	7-9	8-11	8-95
9-10	10-11	11-24	12-13	12-16	12-23	13-14	14-15	15-16	15-17			
16-95	17-18	18-19	18-20	19-22	19-95	20-21	21-22	22-24	57-58			
57-62	58-59	59-60	60-61	61-62	64-65	64-69	65-66	66-67	67-68			
68-69												

exact/norm bonds :

5-95	7-8	8-11	8-95	12-16	13-37	15-16	16-95	19-95	20-36	39-40
40-41	41-73	42-43	43-44	43-74	45-46	45-49	47-48	47-50	47-76	
49-75	51-52	51-77	53-78	54-79	55-81	91-94	92-93	95-105	95-106	

exact bonds :

2-28	3-97	9-96	10-27	14-25	21-26	29-30	31-32	56-57	93-96
94-97									

normalized bonds :

1-2	1-5	1-23	2-3	3-4	4-5	4-6	6-7	7-9	9-10	10-11	11-24	12-13
12-23	13-14	14-15	15-17	17-18	18-19	18-20	19-22	20-21	21-22			
22-24	57-58	57-62	58-59	59-60	60-61	61-62	64-65	64-69	65-66			
66-67	67-68	68-69										

G1: [*1], [*2]

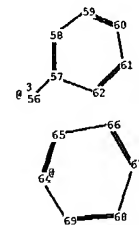
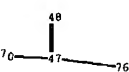
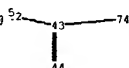
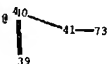
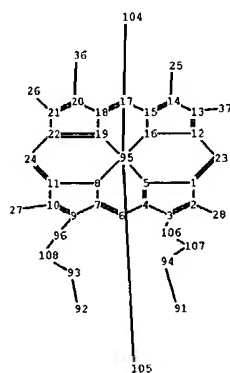
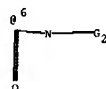
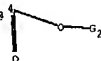
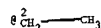
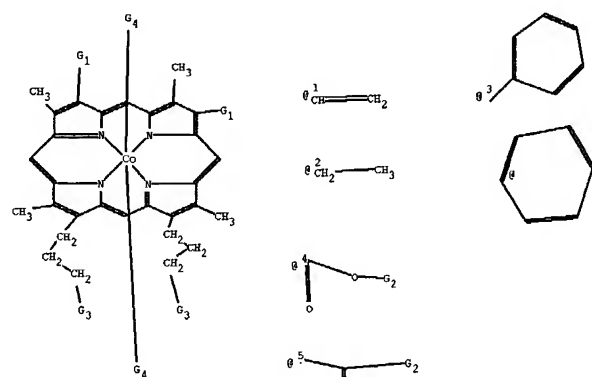
G2: H, CH3, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*2], [*3]

G3: [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11]

G4: X, [*12], [*13], [*14]

Match level :

1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom
10:Atom	11:Atom	12:Atom	13:Atom	14:Atom	15:Atom	16:Atom	17:Atom	
18:Atom	19:Atom	20:Atom	21:Atom	22:Atom	23:Atom	24:Atom	25:Atom	
26:Atom	27:Atom	28:Atom	29:Atom	30:Atom	31:Atom	32:Atom	36:Atom	
37:Atom	39:CLASS	40:CLASS	41:Atom	42:Atom	43:Atom	44:Atom		
45:CLASS	46:CLASS	47:CLASS	48:CLASS	49:CLASS	50:CLASS	51:CLASS		
52:CLASS	53:CLASS	54:CLASS	55:CLASS	56:CLASS	57:Atom	58:Atom		
59:Atom	60:Atom	61:Atom	62:Atom	64:Atom	65:Atom	66:Atom	67:Atom	
68:Atom	69:Atom	73:CLASS	74:CLASS	75:CLASS	76:CLASS	77:CLASS		
78:CLASS	79:CLASS	81:CLASS	91:CLASS	92:CLASS	93:CLASS	94:CLASS		
95:CLASS	96:CLASS	97:CLASS	98:CLASS	99:CLASS	100:CLASS	105:CLASS		
106:CLASS								



N θ^{12}
O θ^{13}
S θ^{14}

97 θ^{12}
98 θ^{13}
99 θ^{14}

chain nodes :

25 26 27 28 29 30 31 32 36 37 39 40 41 42 43 44 45 46
47 48 49 50 51 52 53 54 55 56 73 74 75 76 77 78 79 81
91 92 93 94 96 104 105 106 107 108

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
21 22 23 24 57 58 59 60 61 62 64 65 66 67 68 69 95

ring/chain nodes :

97 98 99

chain bonds :

2-28 3-106 9-96 10-27 13-37 14-25 20-36 21-26 29-30 31-32
39-40 40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50
47-76 49-75 51-52 51-77 53-78 54-79 55-81 56-57 91-94 92-93
93-108 94-107 95-104 95-105 96-108 106-107

ring bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 5-95 6-7 7-8 7-9 8-11 8-95
9-10 10-11 11-24 12-13 12-16 12-23 13-14 14-15 15-16 15-17
16-95 17-18 18-19 18-20 19-22 19-95 20-21 21-22 22-24 57-58
57-62 58-59 59-60 60-61 61-62 64-65 64-69 65-66 66-67 67-68
68-69

exact/norm bonds :

5-95 7-8 8-11 8-95 12-16 13-37 15-16 16-95 19-95 20-36 39-40
40-41 41-73 42-43 43-44 43-74 45-46 45-49 47-48 47-50 47-76
49-75 51-52 51-77 53-78 54-79 55-81 91-94 92-93 95-104 95-105

exact bonds :

2-28 3-106 9-96 10-27 14-25 21-26 29-30 31-32 56-57 93-108
94-107 96-108 106-107

normalized bonds :

1-2	1-5	1-23	2-3	3-4	4-5	4-6	6-7	7-9	9-10	10-11	11-24	12-13
12-23	13-14	14-15	15-17	17-18	18-19	18-20	19-22	20-21	21-22			
22-24	57-58	57-62	58-59	59-60	60-61	61-62	64-65	64-69	65-66			
66-67	67-68	68-69										

G1: [*1], [*2]

G2: H, CH3, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, [*2], [*3]

G3: [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11]

G4: X, [*12], [*13], [*14]

Match level :

1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom
10:Atom	11:Atom	12:Atom	13:Atom	14:Atom	15:Atom	16:Atom	17:Atom	
18:Atom	19:Atom	20:Atom	21:Atom	22:Atom	23:Atom	24:Atom	25:Atom	
26:Atom	27:Atom	28:Atom	29:Atom	30:Atom	31:Atom	32:Atom	36:Atom	
37:Atom	39:CLASS	40:CLASS	41:Atom	42:Atom	43:Atom	44:Atom		
45:CLASS	46:CLASS	47:CLASS	48:CLASS	49:CLASS	50:CLASS	51:CLASS		
52:CLASS	53:CLASS	54:CLASS	55:CLASS	56:CLASS	57:Atom	58:Atom		
59:Atom	60:Atom	61:Atom	62:Atom	64:Atom	65:Atom	66:Atom	67:Atom	
68:Atom	69:Atom	73:CLASS	74:CLASS	75:CLASS	76:CLASS	77:CLASS		
78:CLASS	79:CLASS	81:CLASS	91:CLASS	92:CLASS	93:CLASS	94:CLASS		
95:CLASS	96:CLASS	97:CLASS	98:CLASS	99:CLASS	104:CLASS	105:CLASS		
106:CLASS	107:CLASS	108:CLASS						

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptaul29pxo

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 15:06:15 ON 03 MAY 2004
FILE 'CAPLUS' ENTERED AT 15:06:15 ON 03 MAY 2004
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
COST IN U.S. DOLLARS

	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	5.63	1007.79

	SINCE FILE	TOTAL
	ENTRY	SESSION
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)		
CA SUBSCRIBER PRICE	-0.69	-8.31

=> file reg

	SINCE FILE	TOTAL
	ENTRY	SESSION
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	5.63	1007.79

	SINCE FILE	TOTAL
	ENTRY	SESSION
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)		
CA SUBSCRIBER PRICE	-0.69	-8.31

FILE 'REGISTRY' ENTERED AT 15:06:26 ON 03 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 30 APR 2004 HIGHEST RN 678535-01-8
DICTIONARY FILE UPDATES: 30 APR 2004 HIGHEST RN 678535-01-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\STNEXP4\QUERIES\867h.str

L21 STRUCTURE UPLOADED

=>

Uploading C:\STNEXP4\QUERIES\867g.str

L22 STRUCTURE UPLOADED

=> s 121

SAMPLE SEARCH INITIATED 15:11:05 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 13 TO ITERATE

100.0% PROCESSED 13 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 44 TO 476

PROJECTED ANSWERS: 0 TO 0

L23 0 SEA SSS SAM L21

=> search 121

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.

ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full

FULL SEARCH INITIATED 15:11:12 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 265 TO ITERATE

100.0% PROCESSED 265 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L24 0 SEA SSS FUL L21

=> s 122

SAMPLE SEARCH INITIATED 15:11:20 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 14 TO ITERATE

100.0% PROCESSED 14 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 56 TO 504

PROJECTED ANSWERS: 0 TO 0

L25 0 SEA SSS SAM L22

=> search 122

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.

ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full

FULL SEARCH INITIATED 15:11:28 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 241 TO ITERATE

100.0% PROCESSED 241 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L26 0 SEA SSS FUL L22